National Aeronautics and Space Administration

# HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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# Aitken Expansion Completes First MSF Compute Module

- HECC's Systems team completed the new Aitken expansion and placed the system into production—further increasing Aitken's compute capability by 22%, from 10.76 petaflops (PF) to 13.12 PF.
- The expansion completes the installation of compute resources in the first Aitken module located on the one-acre site of the Modular Supercomputing Facility (MSF).
- The expansion comprises 512 Apollo 9000 "Badger" nodes.
  - Each node has two 64-core AMD second-generation System-on-Chip (SoC) EPYC (pronounced "epic") 7742 Rome processors.
  - This adds an additional 65,536 cores and 262 terabytes memory.
- The HPE Performance Cluster Manager (HPCM) is used to manage the cluster configuration.
- The new nodes use the Portable Batch System (PBS) scheduler and expand the existing InfiniBand fabric within Aitken.

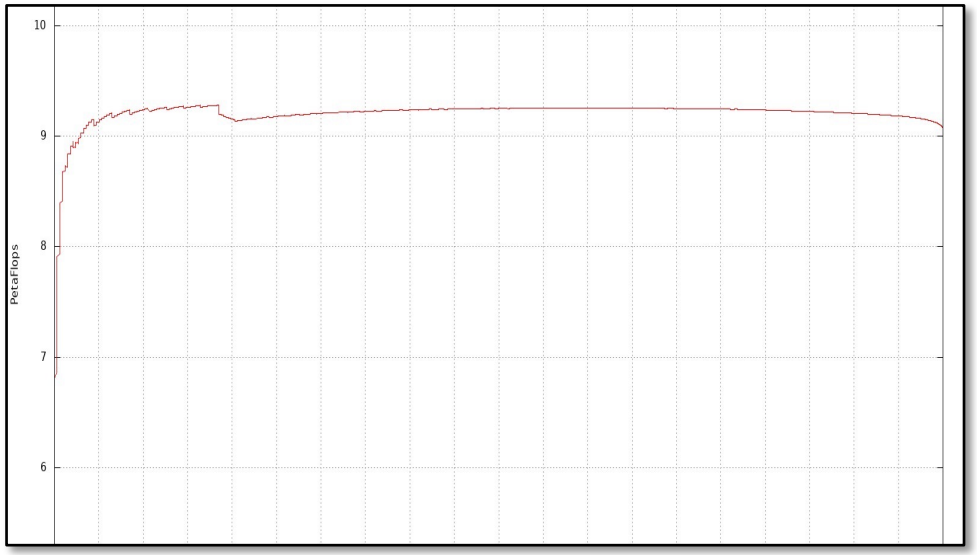
**IMPACT**: The Aitken supercomputer expansion provides more computing capacity and resources to support research engineers and scientists for NASA mission projects.


The first module of the Modular Supercomputing Facility at NASA Ames houses the Aitken supercomputer. The one-acre site can potentially hold 16 modules for both computing and data systems. *Derek Shaw, NASA/Ames*

# Expanded Aitken System is Successfully Benchmarked

- HECC system administrators ran the LINPACK and High-Performance Conjugate Gradients (HPCG) benchmarks on the newly expanded Aitken supercomputer to measure its performance and identify any faulty components prior to releasing the system for general user availability.
  - The system achieved 9.07 petaflops (PF) on the LINPACK benchmark and 172.375 teraflops (TF) on the HPCG benchmark.
  - If the results had been included in the November 2021 TOP500 and HPCG lists, the system would have ranked #54 on the TOP500 and #40 on the HPCG list.
- These benchmarks, acting as diagnostic tests on the full system, identified a hardware component with marginal performance, which as a result was replaced prior to further integration and testing.
- The LINPACK and HPCG benchmarks are widely used to evaluate the performance of different supercomputing systems and provide two complementary viewpoints on how systems perform on different workloads.

**IMPACT**: HECC regularly upgrades its resources to meet NASA's growing supercomputing requirements and increase the rate at which science and engineering results are generated. Running the LINPACK and HPCG benchmarks on expanded systems provides a good method to identify and address system issues, thereby improving overall reliability for users.

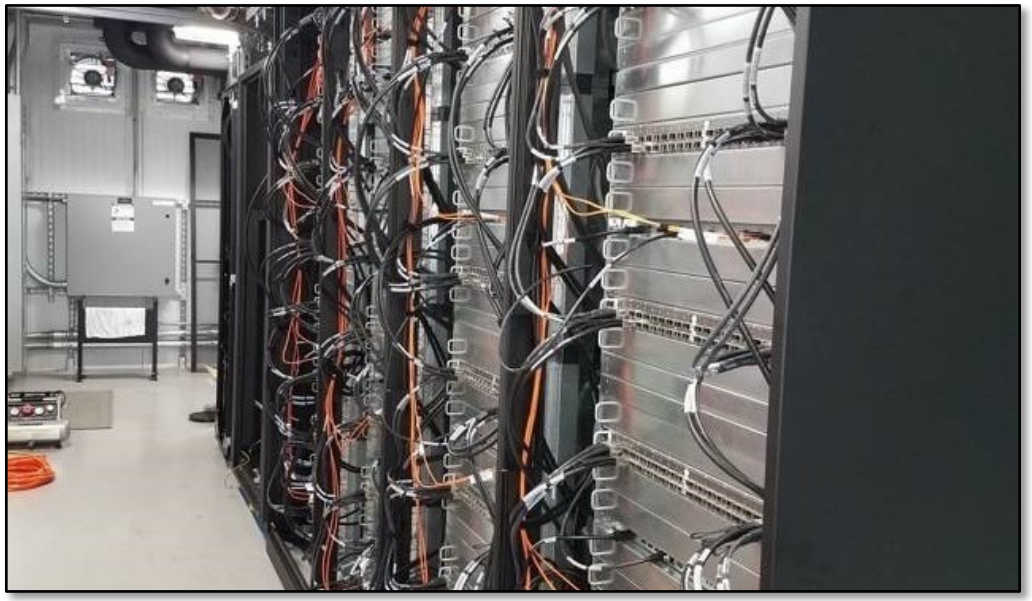



This chart shows the 11-hour successful LINPACK benchmark run on the Aitken supercomputer. *Greg Matthews, NASA/Ames*

# Recabling of the Aitken Long-Distance InfiniBand

- HECC's Supercomputing Systems team completed recabling of the long-distance InfiniBand (IB) network connections between the Aitken supercomputer housed in the Modular Supercomputing Facility (MSF) and the main NAS facility (Building N258) at Ames.
- Aitken depends on these long-distance connections for access to filesystems and critical infrastructure components, such as the Portable Batch System job scheduler.
- The new cabling is an improvement in three key aspects:
  - Reliability: The cabling removes single points of failure that resulted in Aitken downtime in the past.
  - Efficiency: Fewer IB switches and cables are required for the new cabling, freeing up four IB switches and dozens of cables for other uses.
  - Distance: The new cabling utilizes shorter-distance underground fiber pulled between Aitken and N258.
- The Systems team will utilize the cables as a foundation for future expansion of Aitken and will continue to investigate IB capability upgrades that improve these long-distance connections.

**IMPACT**: Network recabling improves the reliability of the Aitken supercomputer and allows more efficient use of HECC's investment in InfiniBand high-performance networking communications.

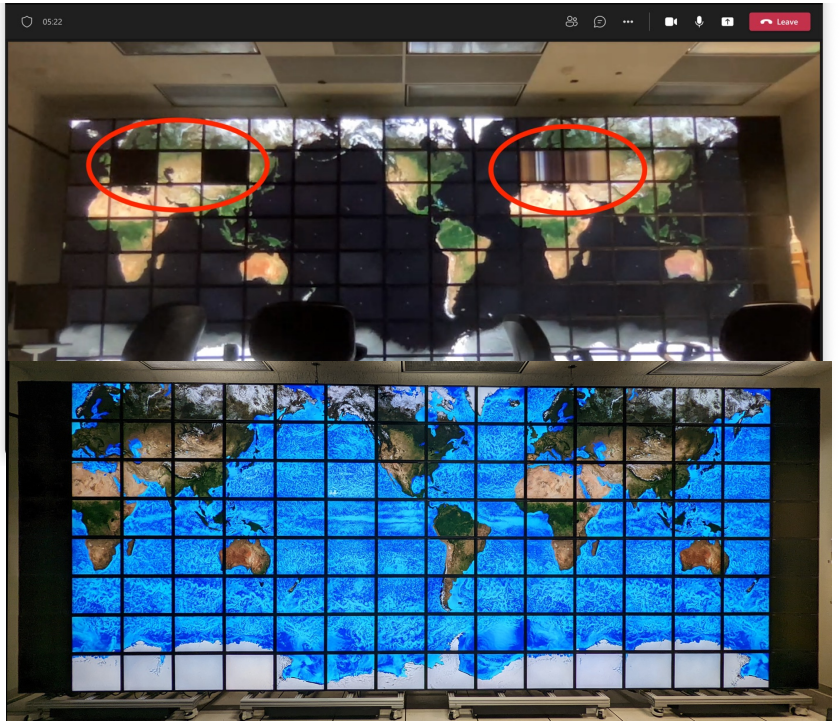


Back panels removed from the Aitken AMD Apollo 9000 Badger racks show a portion of the InfiniBand cabling that provides high-performance network connectivity. *Image credit: HPE*

# NAS hyperwall Maintenance Allows Continued VIP Demos

- The hyperwall visualization system at the NASA Advanced Supercomputing (NAS) facility is a key stop for demonstrating science and engineering work done at NASA Ames, where VIP tours have resumed as part of the Center's return-to-work plan.
- The hyperwall's 128 monitors are nearly 15 years old and failing regularly. The current failure rate is about two monitors per month. The last spare monitor was used before the pandemic started.
- To solve this problem, the HECC Visualization team deactivates columns of monitors and uses them as spares. Two columns of monitors have been deactivated so far.
- The team modified the demonstration layout script so it can automatically adjust layouts by removing the deactivated columns. This approach facilitated at least five successful demos for visitors without visible monitor failures.
- Continued maintenance will allow VIP demos until the monitors are removed for the upcoming Visualization Lab renovation. The project to upgrade the hyperwall room and monitors is in the bid walkthrough phase.
- Recent VIPs include ARMD Associate Administrator Bob Pearce, and Science Mission Directorate Astrophysics leaders.

**IMPACT**: Maintenance efforts allow important visitors at NASA Ames to continue receiving effective demonstrations highlighting results computed on HECC systems.

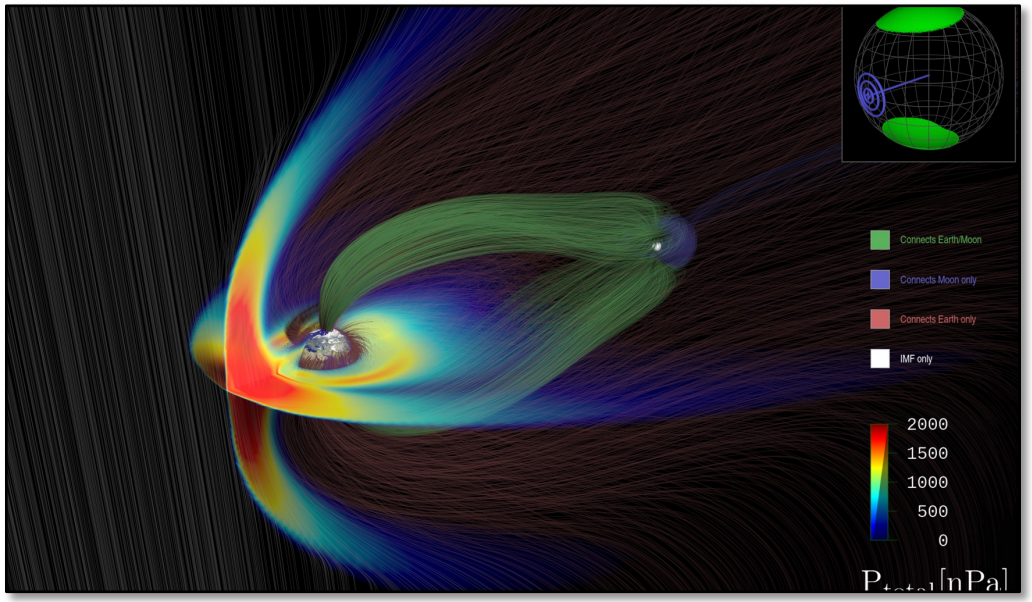


Top: Screenshot of the hyperwall with four failed monitors (circled) and one deactivated column. Bottom: The hyperwall with the failed monitors relocated to the now-deactivated left column.
*David Ellsworth, NASA/Ames*

# Visualizing Mechanisms for Making Water on the Moon

- The HECC Data Analysis and Visualization Group produced images and animations supporting Princeton University researchers' challenging effort to trace the origin of lunar water. The work illustrates a possible mechanism for Lunar hydration: ionized oxygen transported by Earth's magnetic field.
- The HECC team applied adaptive vector field tracing, which allowed oxygen ion footprint generation.
  - Densely seeded magnetic field lines on each sphere did not initially fill the footprints, producing spotty results. An adaptive routine was written to seed regions around existing field lines to fill in the gaps.
- The animations help convey a dynamic system of ionized oxygen deposition.
  - Magnetic field lines and footprints of possible deposition are shown.
  - Cutting planes show the deflection of the solar wind by Earth's magnetic field, shielding the transport of oxygen ions.
  - Animating the view helps convey a mental model of the 3D system. Connection and scalar keys describe the visual elements in the scene.
- The visualizations give insight into supercomputer-generated data, helping scientists express their complex computational results.

**IMPACT**: Visualizations provided by HECC experts enhance our understanding of complex physics and contribute to NASA's plan for sustained lunar exploration and development.




Magnetic field lines, shown in green, provide a pathway from the Earth to the Moon for oxygen ions, a possible contributor to lunar hydration. The footprint key in the upper right corner shows potential lunar deposition sites in green, with a blue glyph indicating Earth's direction. *Tim Sandstrom, NASA/Ames; Chuanfei Dong, Princeton University*

# Applications Team Runs SBU2 Benchmarks on New NCCS Discover Cascade Lake Nodes

- HECC's Application Performance and Productivity (APP) team recently ran the SBU2 benchmark suite on the NASA Center for Climate Simulation (NCCS) Discover system's new Scalable Unit 16 (SCU16) Cascade Lake nodes.
  - SCU16 holds 676 nodes connected with Mellanox (Nvidia) HDR100 InfiniBand, unlike SCU14 and SCU15 (Skylake) nodes, which uses Intel Omni-Path.
  - Each SCU16 node has 190 gigabytes (GB) total memory and 48 cores, with a maximum of 46 cores available for user jobs.
- Most of the SBU2 tests ran without issue. APP did encounter some difficult issues running USM3D with Intel MPI on SCU16.
  - NCCS support staff provided extensive assistance with USM3D.
  - USM3D ran to completion on Skylake nodes without issue using the recommended Intel MPI and Intel compiler. This could not be replicated on Cascade Lake nodes, even with a reduced core count.
  - USM3D only ran to completion after using Mellanox (Nvidia) HPCX MPI and reducing the core count to 44 per node (which was accounted for in the final SBU2 rate). NCCS suggests this could be an InfiniBand-specific issue with Intel MPI.
- The APP team provided a final SBU2 rate of 1.77 to NCCS for the SCU16 nodes.

** SBU2 rate of 1.0 is 1 hour on one Broadwell node*

**IMPACT**: Using a common Standard Billing Unit (SBU) metric for High End Computing Program resources helps balance user demand on different resource types and gives management a way to compare supercomputing resource usage among the mission directorates.


The centerpiece of the NASA Center for Climate Simulation (NCCS) computing resources is the over 129,000-core "Discover" supercomputing cluster, an assembly of multiple Linux scalable units built upon commodity components. The newest scalable unit is SCU16. *NASA*

# 97% Reduction in Control Room New Hire Access Time

- The HECC User Services and Network teams worked collaboratively to update the onboarding process for NAS Control Room (CR) new hires, reducing the time required for employees to access resources needed to perform CR tasks from two months to two days.
- Control Room analysts (CRAs) evaluated the onboarding process, identified areas for improvement, and implemented:
  - The Control Room originally used workstations, which required PIV cards to log on. Workstations required PIV card access (~3 months to process).
  - CRAs transitioned from workstations to Macs, where new hires can sign-on without a PIV card under a temporary PIV exception. The Networks team supplied LAN connections for each Mac.
  - Ethernet connections in the Control Room enable new staff members to be more productive by having immediate, limited access to non-sensitive internal tools such as Remedy and internal wikis.
  - New-hire curriculum now allows for independent training.
- These changes have allowed new hires to become productive team members within a few weeks rather than months.

**IMPACT**: Updated processes enable significant reduction in onboarding time for new hires to the Control Room, which increases productivity and improves new-hire morale.


*Free stock image*

# CFD Analysis of the Transonic Truss-Braced Wing Aircraft*

- The Boeing Transonic Truss-Braced Wing (TTBW) concept has the potential to improve fuel efficiency of commercial aircraft. Due to its unconventional configuration, initial CFD analyses were not sufficient to reliably assess its performance. A multi-center effort by the Advanced Air Transport Technology Project was launched to develop new methods to better predict the TTBW's performance.
- Researchers in the NASA Advanced Supercomputing Division's Computational Aerosciences Branch performed simulations using the Launch Ascent and Vehicle Aerodynamics (LAVA) solver and NASA Langley's USM3D. Through comparison of a variety of solvers, grids, and turbulence models, the team was able to show the relative strengths and weaknesses of each model.
- HECC resources made it possible to run the Spalart-Allmaras (SA) models in a short timeframe, and results from initial Sheer Stress Transport (SST) models—which required 37 times the resources as the SA models—were obtained within a week. After optimization, an angle of attack case for the SST models required 8–12 hours on 4,000 cores to get a converged solution.

** HECC provided supercomputing resources and services in support of this work.*

**IMPACT**: Determining the agency's computational modeling capability and establishing best practices will help facilitate aerodynamic design, prediction, and analysis of current and future aircraft concepts.

A wall-modeled large eddy simulation of a Mach=0.8 flow past the TTBW concept aircraft at an angle of attack outside typical cruise conditions. The surface skin friction is shown, and the contour map outlines separated flow on the wing and strut. These simulations used an immersed boundary method on a block-structured Cartesian grid within the LAVA code. *Oliver M. Browne, NASA/Ames*

# Papers

- "**Wall-Modeled Large-Eddy Simulation of Three-Dimensional Turbulent Boundary Layer in a Bent Square Duct**," X. Hu, I. Hayat, G. I. Park, arXiv:2204.00537 [physics.flu-dyn], April 1, 2022. *
  *https://arxiv.org/abs/2204.00537*
- "**A Close-In Puffy Neptune with Hidden Friends: The Enigma of TOI 620**," M. Reefe, et al., arXiv:2204.03108 [astro-ph.EP], April 6, 2022. *
  *https://arxiv.org/abs/2204.03108*
- "**Strong Reconnection Electric Fields in Shock-Driven Turbulence**," N. Bessho, et al., Physics of Plasmas, vol. 29, issue 4, published online April 8, 2022. *
  *https://aip.scitation.org/doi/full/10.1063/5.0077529*
- "**The Refined Transit Ephemeris of TOI-2180 b**," P. Dalba, et al., Research Notes of the American Astronomical Society, vol. 6, no. 4, April 2022. *
  *https://iopscience.iop.org/article/10.3847/2515-5172/ac64fd/meta*
- "**Ninety-Seven Eclipsing Quadruple Star Candidates Discovered in TESS Full-Frame Images**," V. Kostov, et al., The Astrophysical Journal Supplement Series, vol. 259, no. 2, April 13, 2022. *
  *https://iopscience.iop.org/article/10.3847/1538-4365/ac5458/meta*
- "**Observed Extra Mixing Trends in Red Giants are Reproduced by the Reduced Density Ratio in Thermohaline Zones**," A. Fraser, et al., arXiv:2204.08487 [astro-ph.SR], April 18, 2022. *
  *https://arxiv.org/abs/2204.08487*

** HECC provided supercomputing resources and services in support of this work.*

# Papers (cont.)

- "**Polar Vortex Crystals: Emergence and Structure**," L. Siegelman, et al., Earth, Atmospheric, and Planetary Sciences, vol. 119, no. 17, April 19, 2022. *
  *https://www.pnas.org/doi/abs/10.1073/pnas.2120486119*
- "**Explicit IMF *By*-Dependence of Energetic Protons and the Ring Current**," L. Holappa, N. Buzulukova, Geophysical Research Letters, vol. 49, issue 8, April 28, 2022. *
  *https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022GL098031*
- "**A Warm Super-Neptune around the G-Dwarf Star TOI-1710 Revealed with TESS, SOPHIE and HARPS-N**," P.-C. Koing, et al., arXiv:2204.08984 [astro-ph.EP], April 19, 2022. *
  *https://arxiv.org/abs/2204.08984*
- "**The HD 260655 System: Two Rocky Worlds Transiting a Bright M-Dwarf at 10 pc**," R. Luque, et al., arXiv:2204.10261 [astro-ph.EP], April 21, 2022. *
  *https://arxiv.org/abs/2204.10261*
- "**GEOM, Energy-Annotated Molecular Conformations for Property Prediction and Molecular Generation**," S. Axelrod, R. Gomez-Bombarelli, Scientific Data, vol. 9, April 21, 2022. *
  *https://www.nature.com/articles/s41597-022-01288-4*
- "**Numerical Simulations of Convective Three-Dimensional Red Supergiant Envelopes**," J. Goldberg, Y.-F. Jiang, L. Bildsten, The Astrophysical Journal, vol. 929, no. 2, April 25, 2022. *
  *https://iopscience.iop.org/article/10.3847/1538-4357/ac5ab3/meta*

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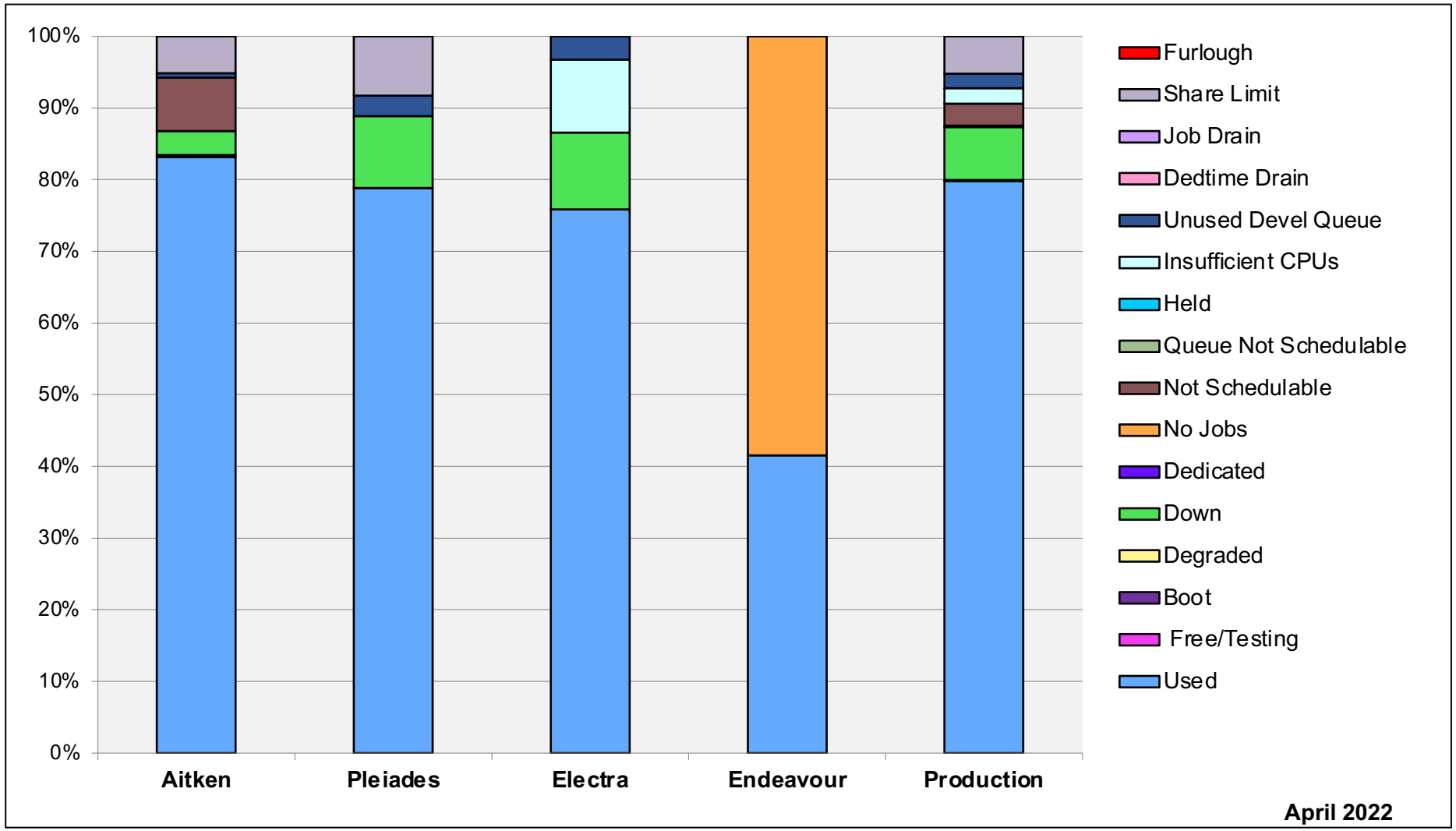
# News and Events

- **X-59 Quiet SuperSonic Technology Aircraft Involves Many Different NASA Facilities,** *Aerotech News*, April 5, 2022—NASA's X-59 experimental aircraft is bringing the agency ever closer to making the quiet commercial supersonic travel over land a reality. Work includes Ames-developed high-resolution, 3D simulation software on the Pleiades, Electra, and Endeavour supercomputers.
  *https://www.aerotechnews.com/blog/2022/04/04/x-59-quiet-supersonic-technology-aircraft-involves-many-different-nasa-facilities/*
- **NASA Spotlights Its Galaxy of HPC Activities**, *HPCwire*, April 15, 2022— "HPC Matters!" was the big, bold title of a talk by Piyush Mehrotra, division chief of NASA's Advanced Supercomputing (NAS) Division at Ames Research Center, during the meeting of the HPC Advisory Council at Stanford University last week. HPCwire Editor Oliver Peckham covered details of the talk, where Mehrotra offered a glimpse into the state of supercomputing at NASA—and how its systems are being applied to agency missions.
  *https://www.hpcwire.com/2022/04/15/nasa-spotlights-its-galaxy-of-hpc-activities/*
- **HPC Students and NASA Mentors: A Winning Combination**, *NAS Feature*, April 21, 2022—Talented students from diverse communities around the U.S. gained hands-on experience in supercomputing in the second annual Winter Classic Invitational Student Cluster Competition, with help from high-performance computing (HPC) experts in the NASA Advanced Supercomputing (NAS) Division at NASA's Ames Research Center.
  *https://www.nas.nasa.gov/pubs/stories/2022/feature_student_supercomputing_competition.html*
  - **NASA Mentors Students to Achieve High Performance in Supercomputing Competition**, *NASA Ames*, April 28, 2022.
    *https://www.nasa.gov/feature/ames/nasa-mentors-students-to-achieve-high-performance-in-supercomputing-competition*
- **From Supercomputers to Symbiotes, NASA in Silicon Valley Invests in the Earth**, *NASA Ames*, April 22, 2022—On Earth Day, NASA Ames highlights programs that are helping to understand, mitigate, and prepare for Earth's changing climate. The Modular Supercomputing Facility takes advantage of the local climate to cool the Aitken and Electra systems that help scientists make new discoveries about our planet.
  *https://www.nasa.gov/feature/ames/from-supercomputers-to-symbiotes-nasa-in-silicon-valley-invests-in-the-earth*

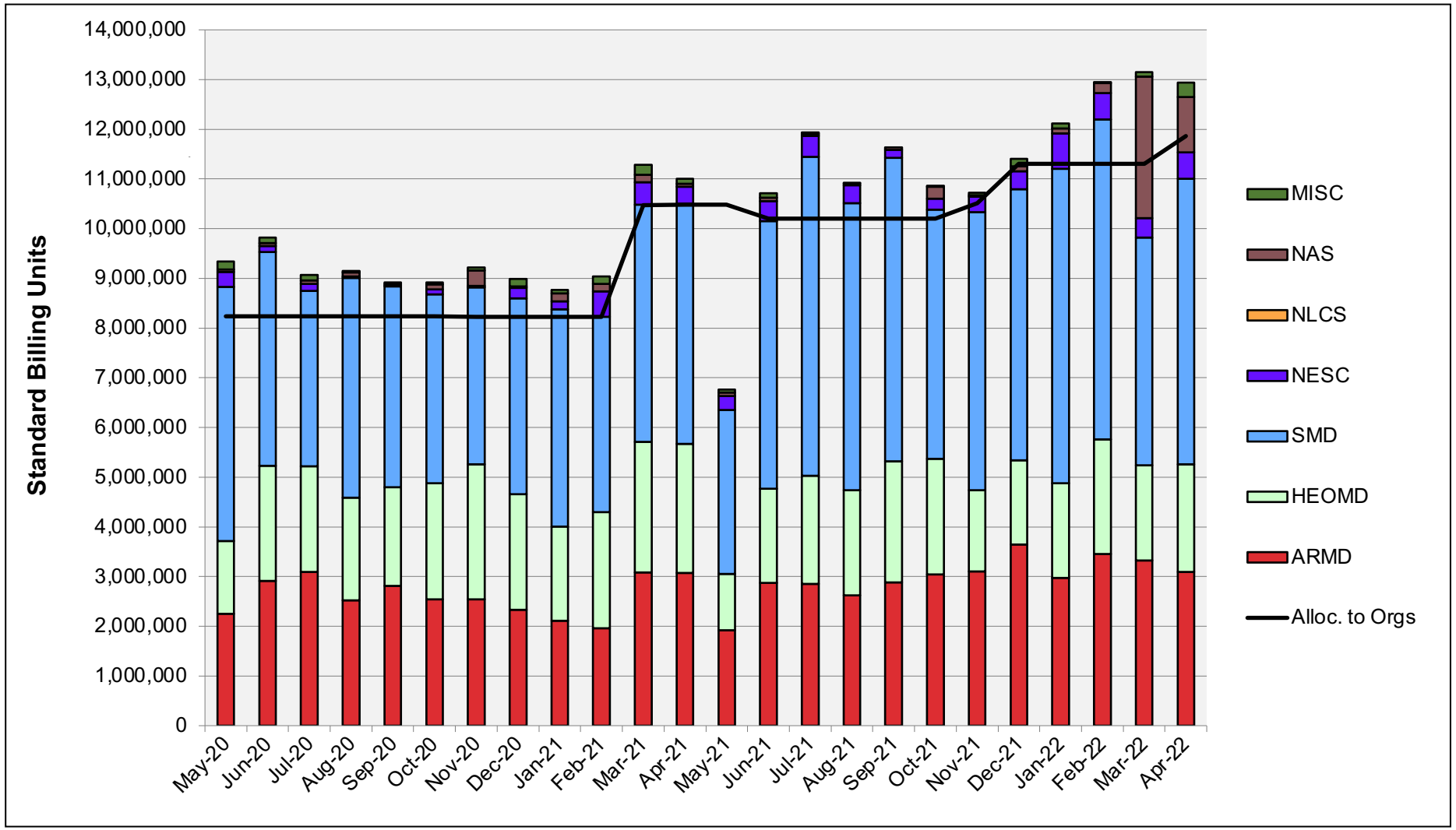
# News and Events: Social Media

- **Coverage of NAS Stories**
  - Topic: Piyush Mehrotra Interview/Talk
    - NAS: Twitter 3 likes.
    - HPCwire: Twitter 3 quote tweets, 4 likes.
  - Topic: Earth Day
    - NAS: Twitter 4 likes.
    - NASA Ames: Twitter 27 retweets, 4 quote tweets, 126 likes.
  - Topic: Winter Classic Student Cluster Competition
    - NAS: Twitter 2 retweets, 3 likes.
    - NASA Ames: Twitter 5 retweets, 26 likes; Facebook 43 likes, 8 shares.

# HECC Utilization



# HECC Utilization Normalized to 30-Day Month



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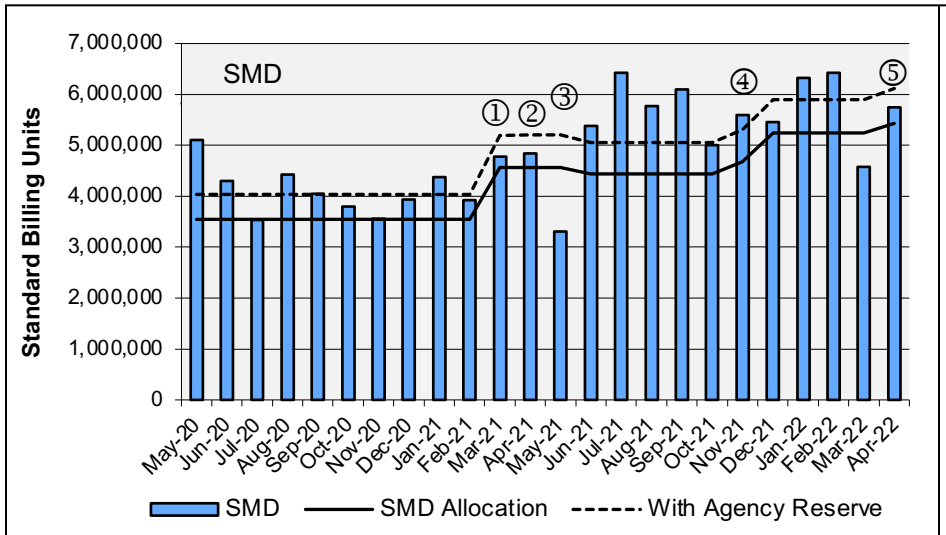
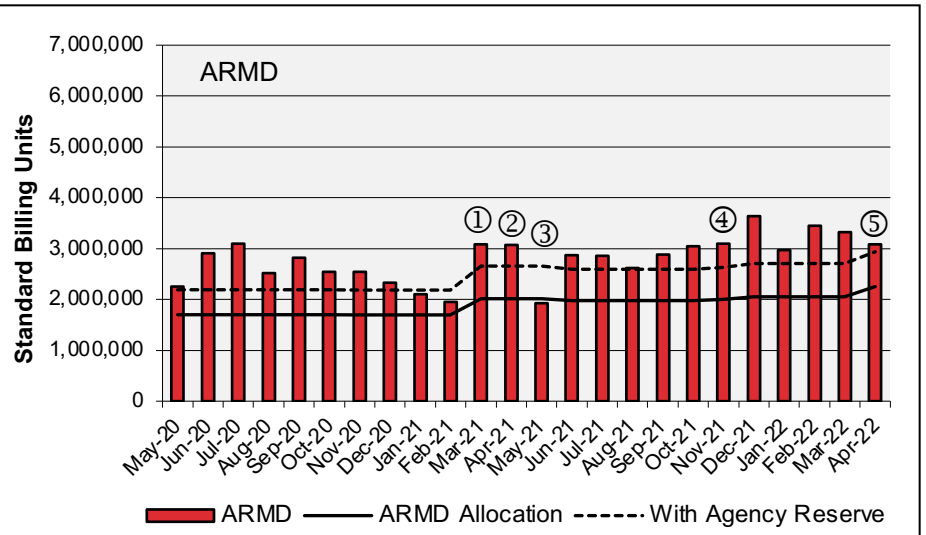
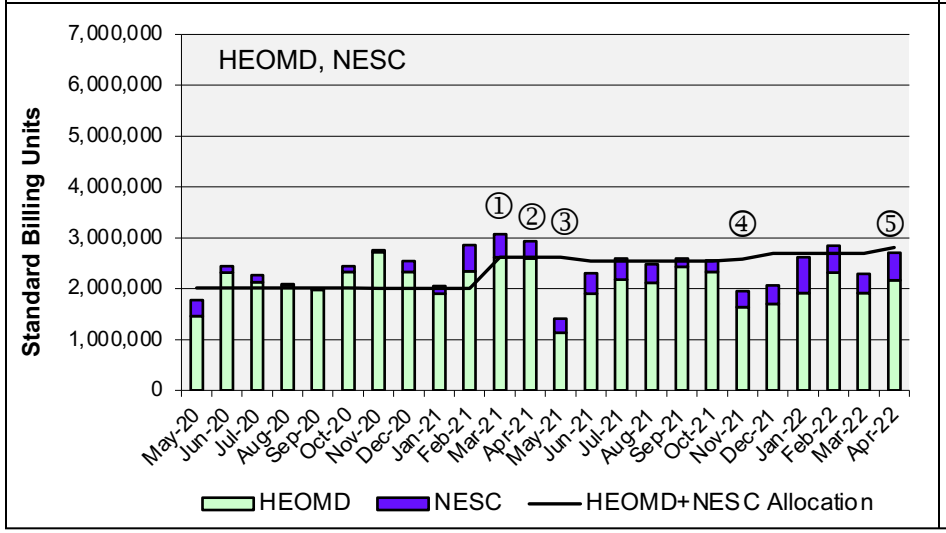



① 8 Rome Apollo racks introduced into Aitken

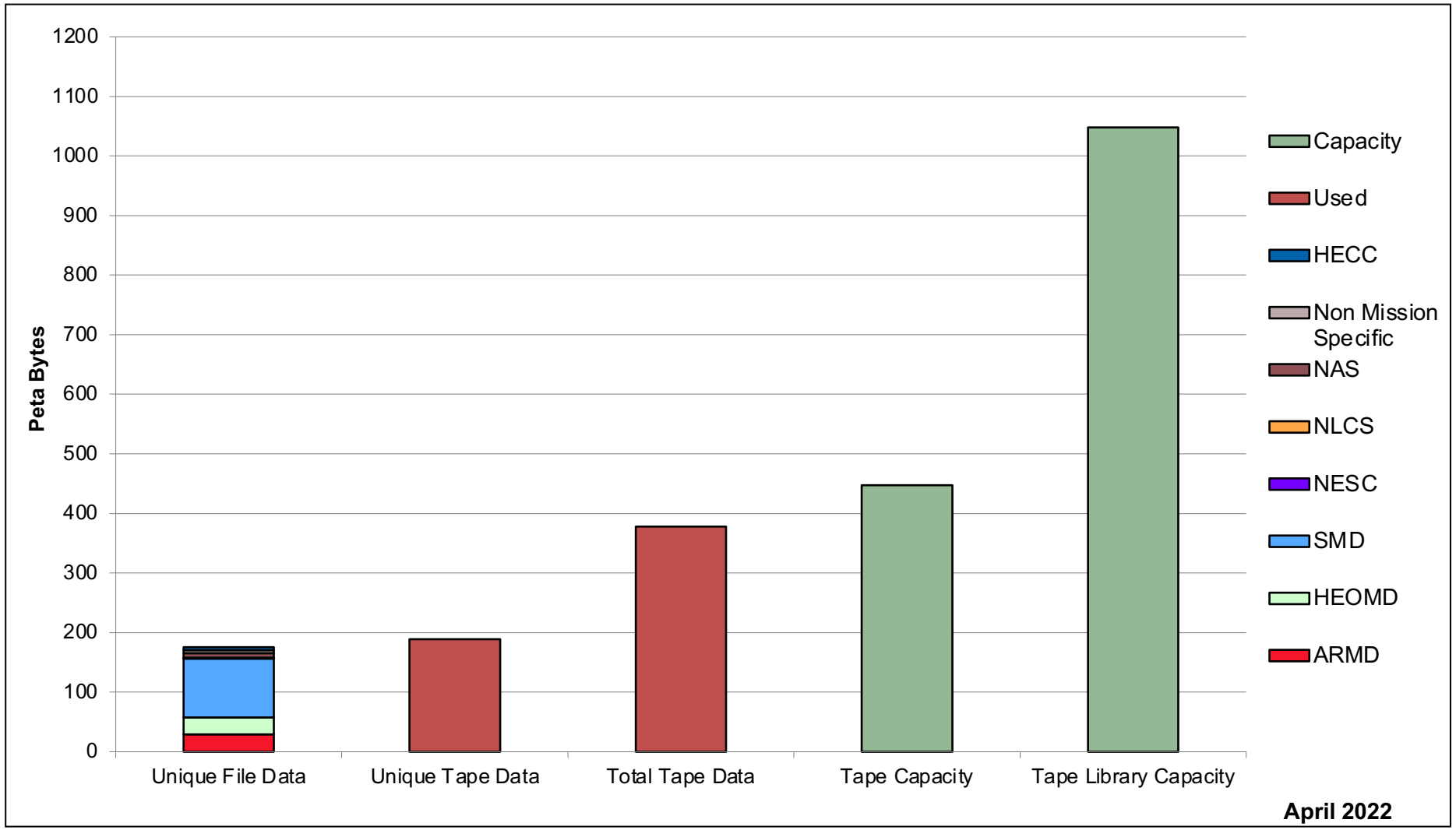
② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

# Tape Archive Status



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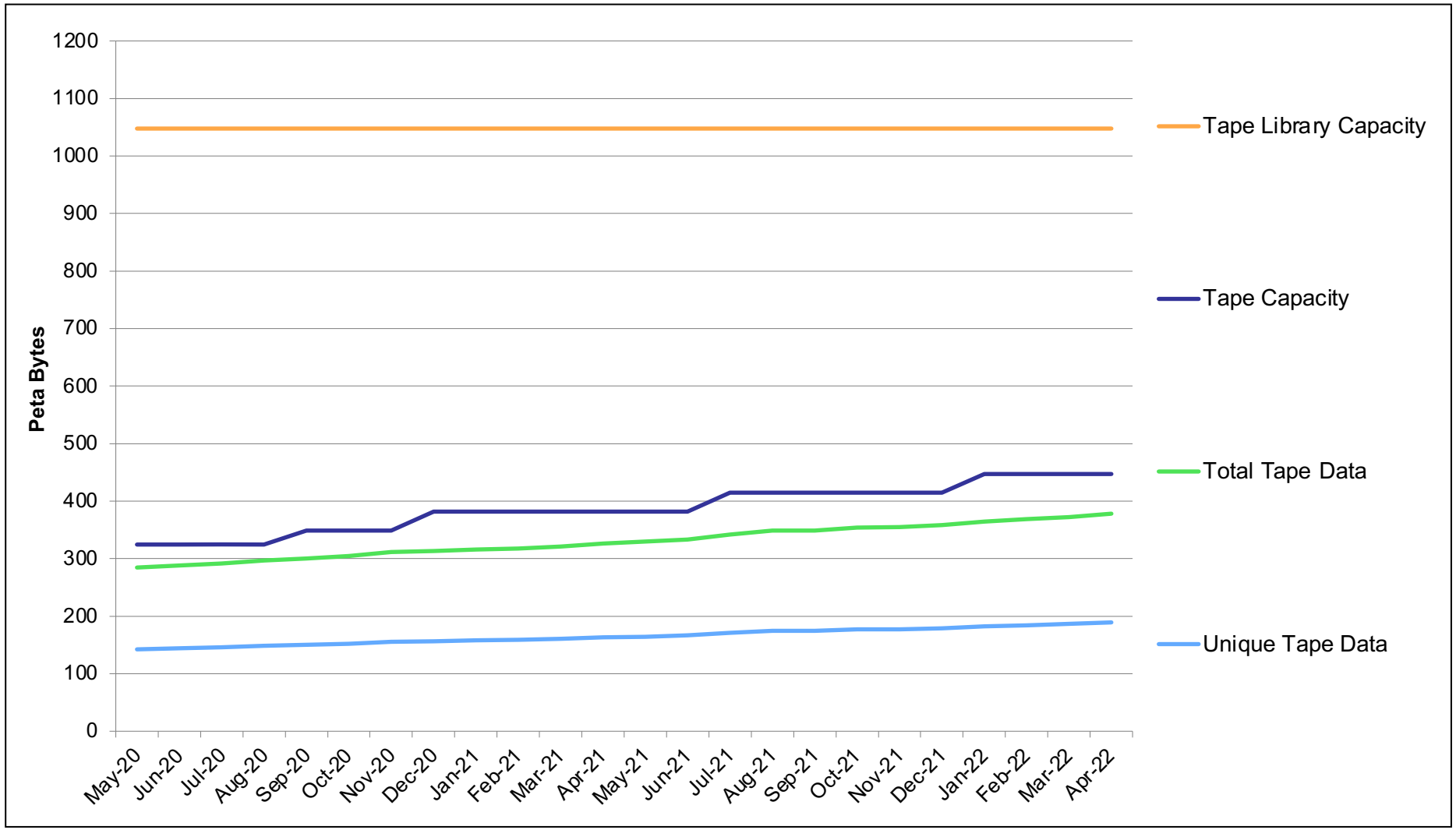
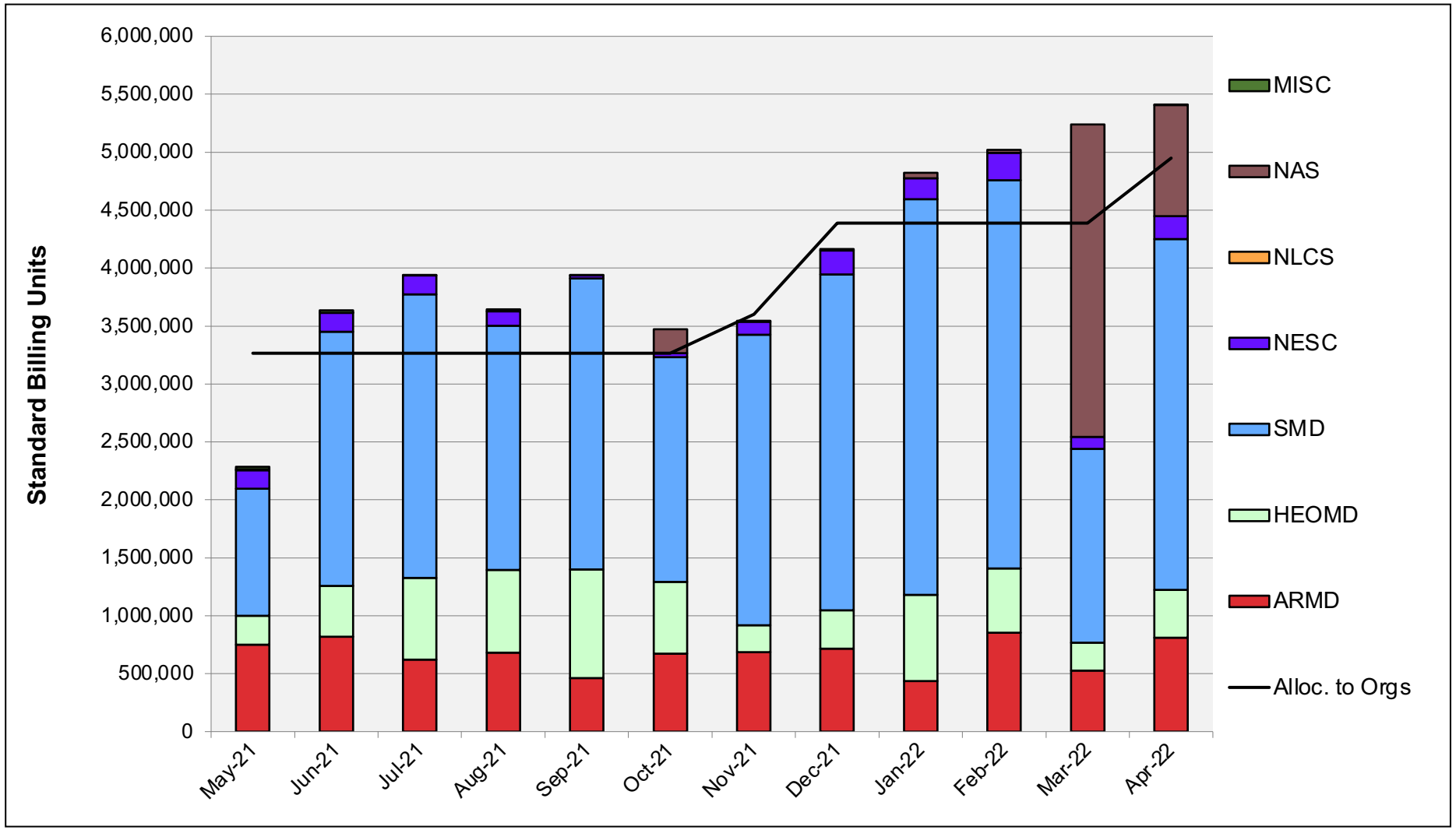
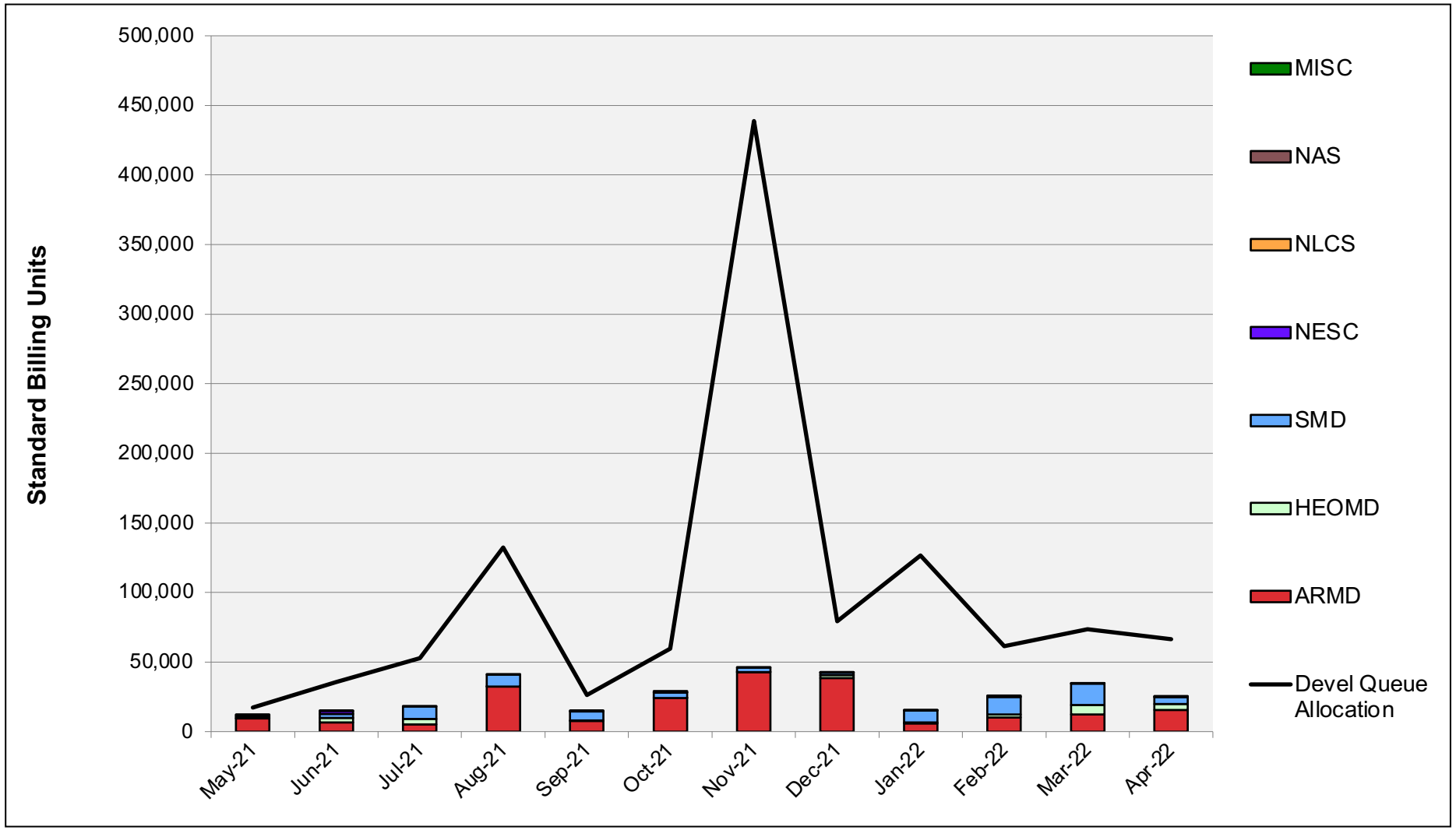


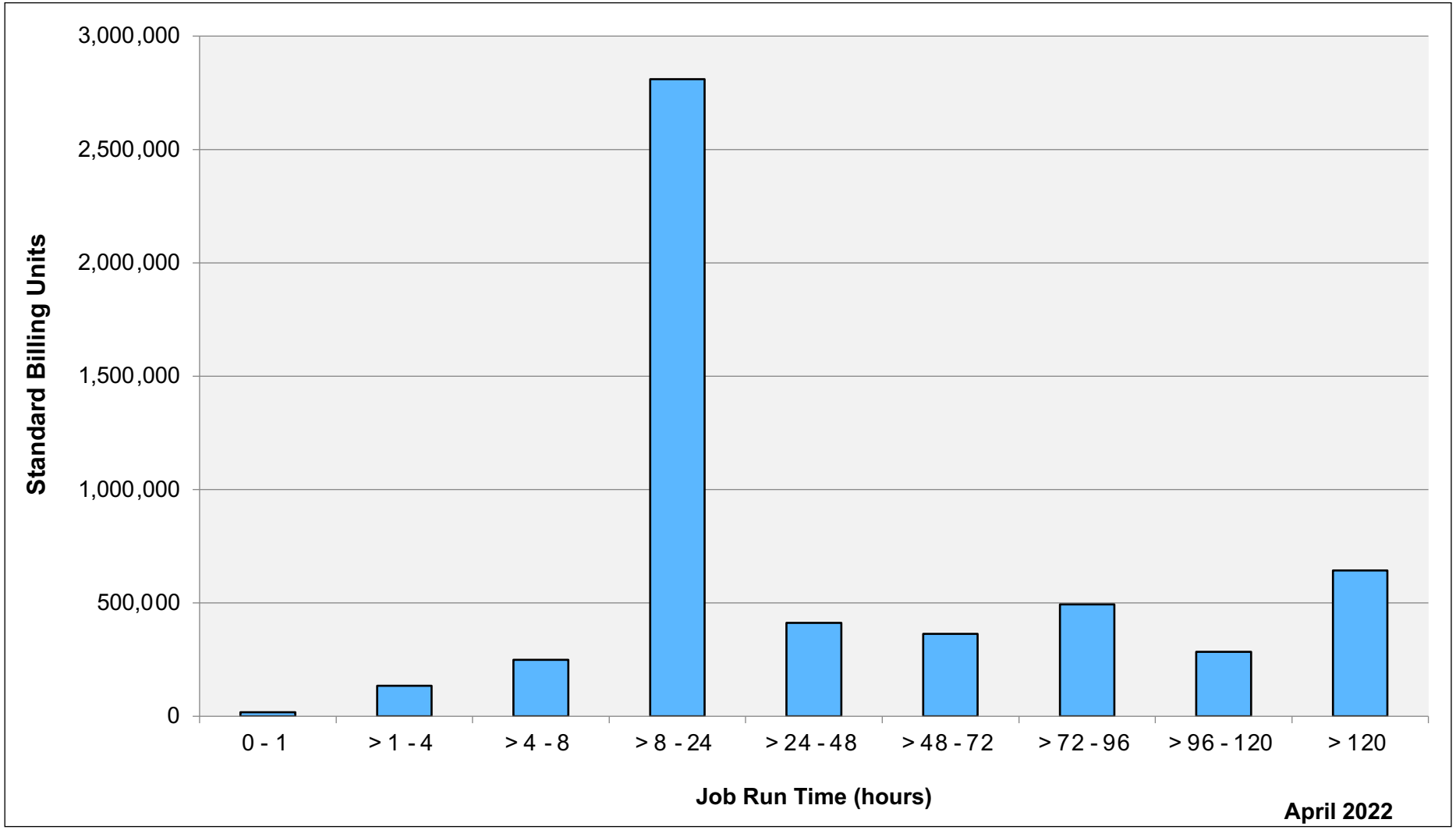
# Aitken: SBUs Reported, Normalized to 30-Day Month



# Aitken: Devel Queue Utilization



# Aitken: Monthly Utilization by Job Length



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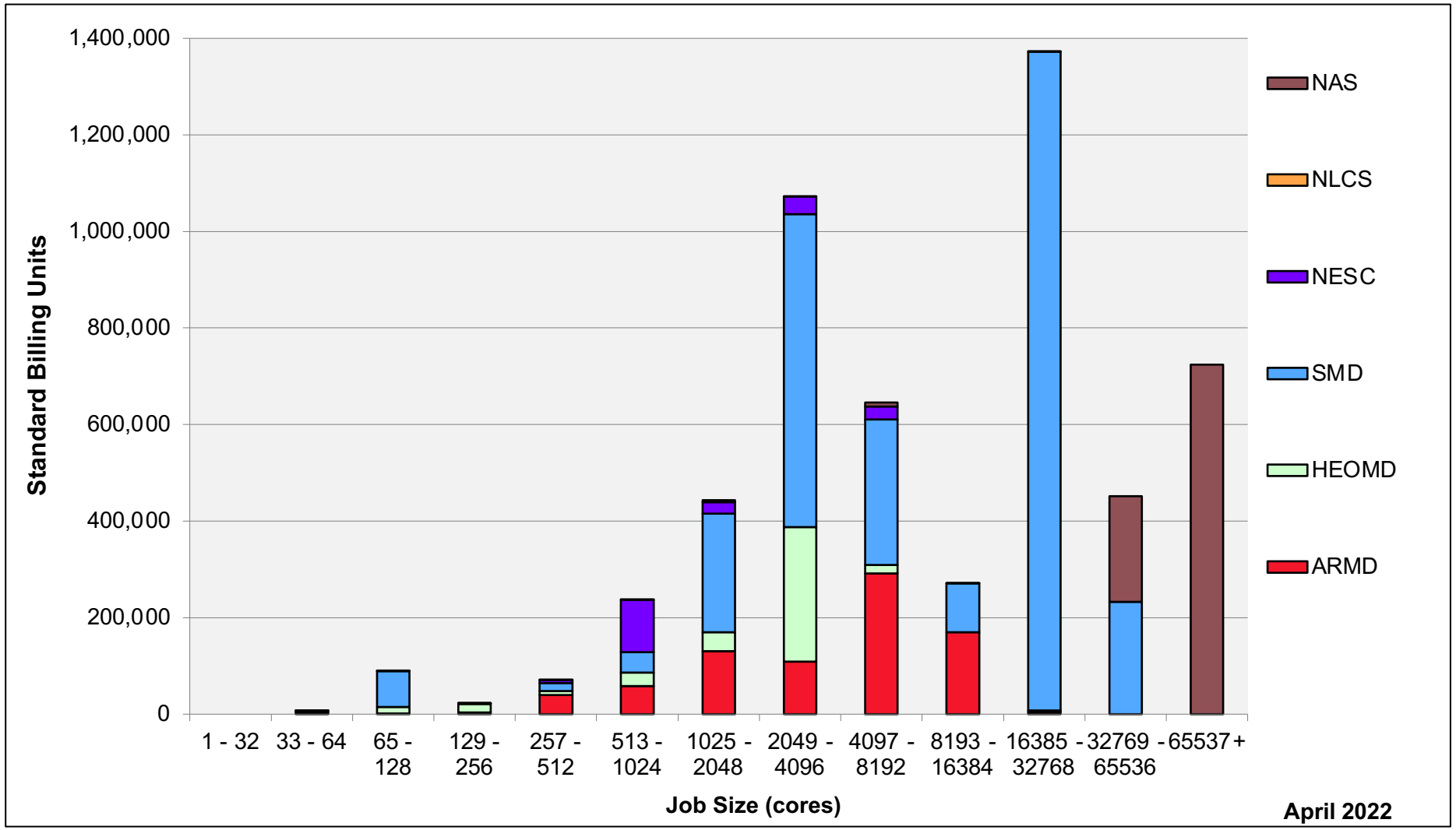
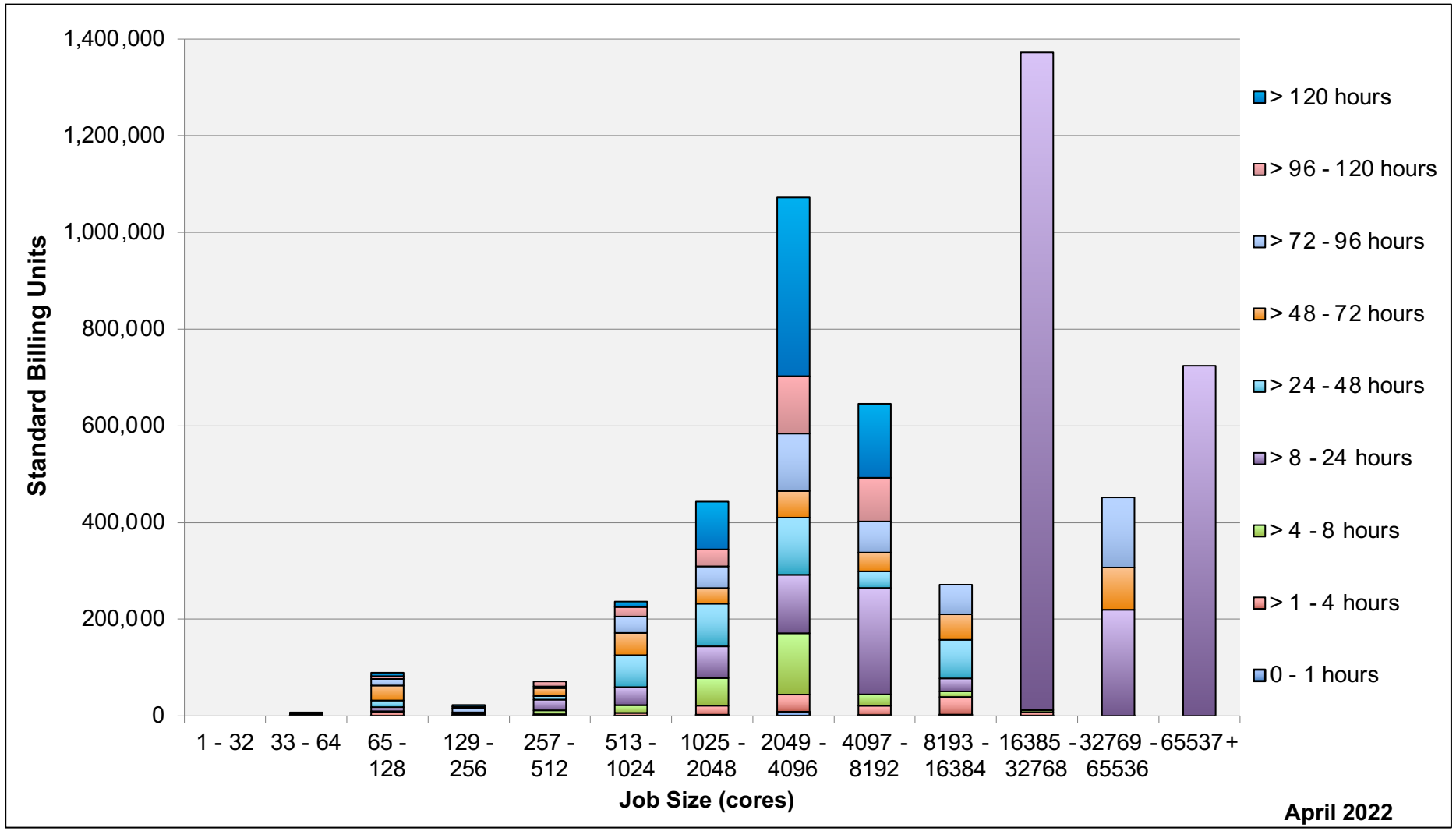
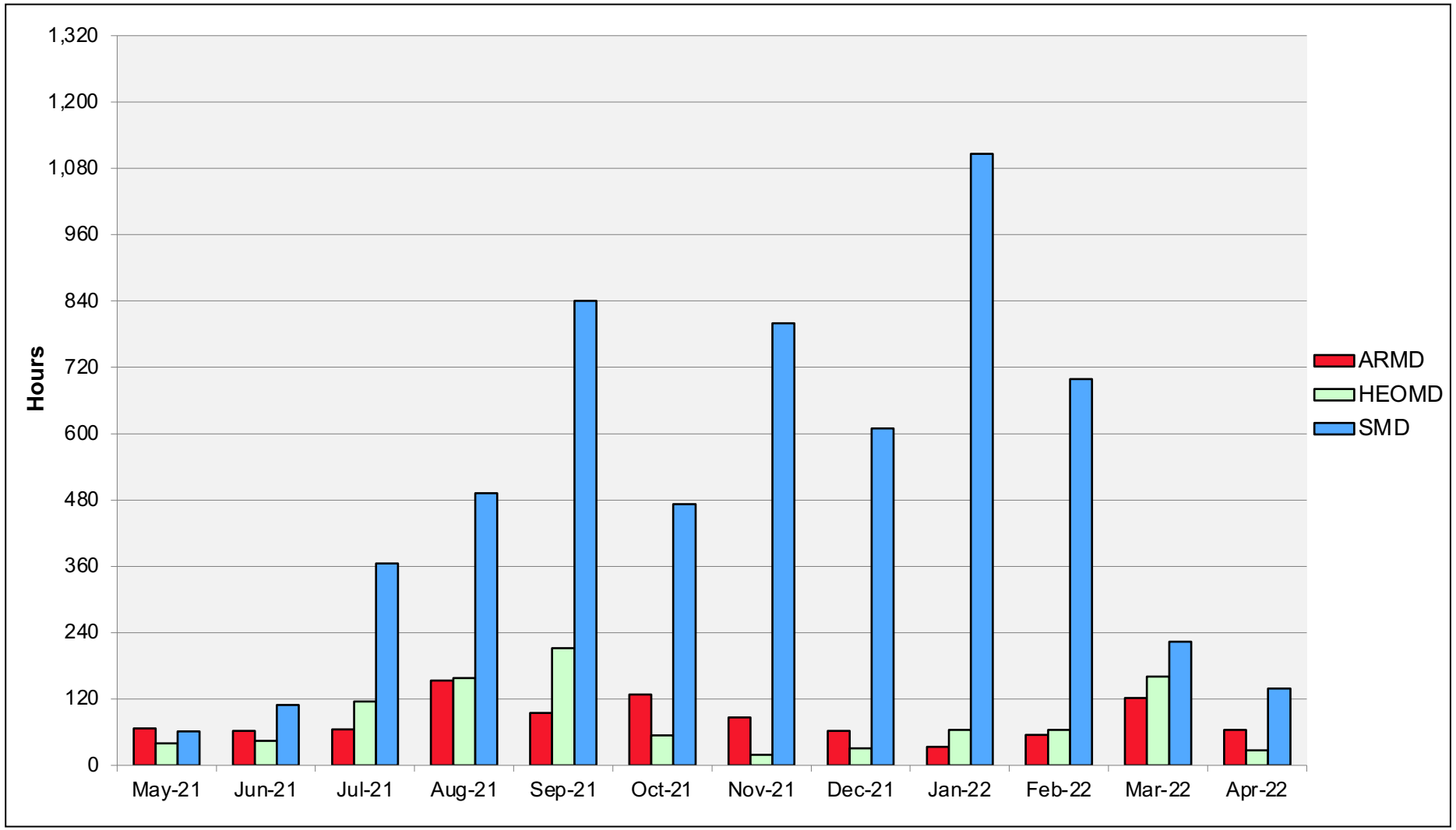


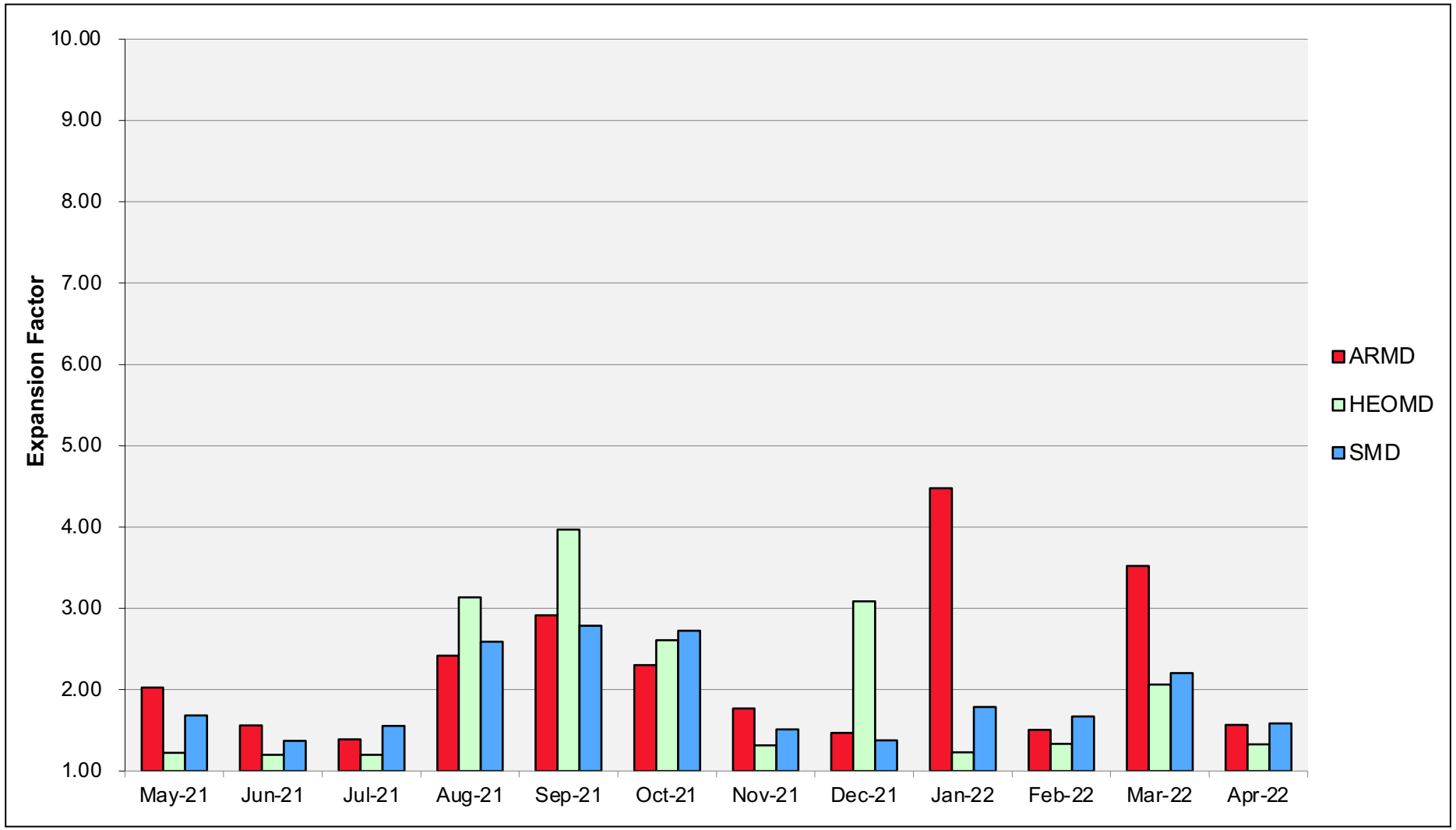
# Aitken: Monthly Utilization by Size and Length



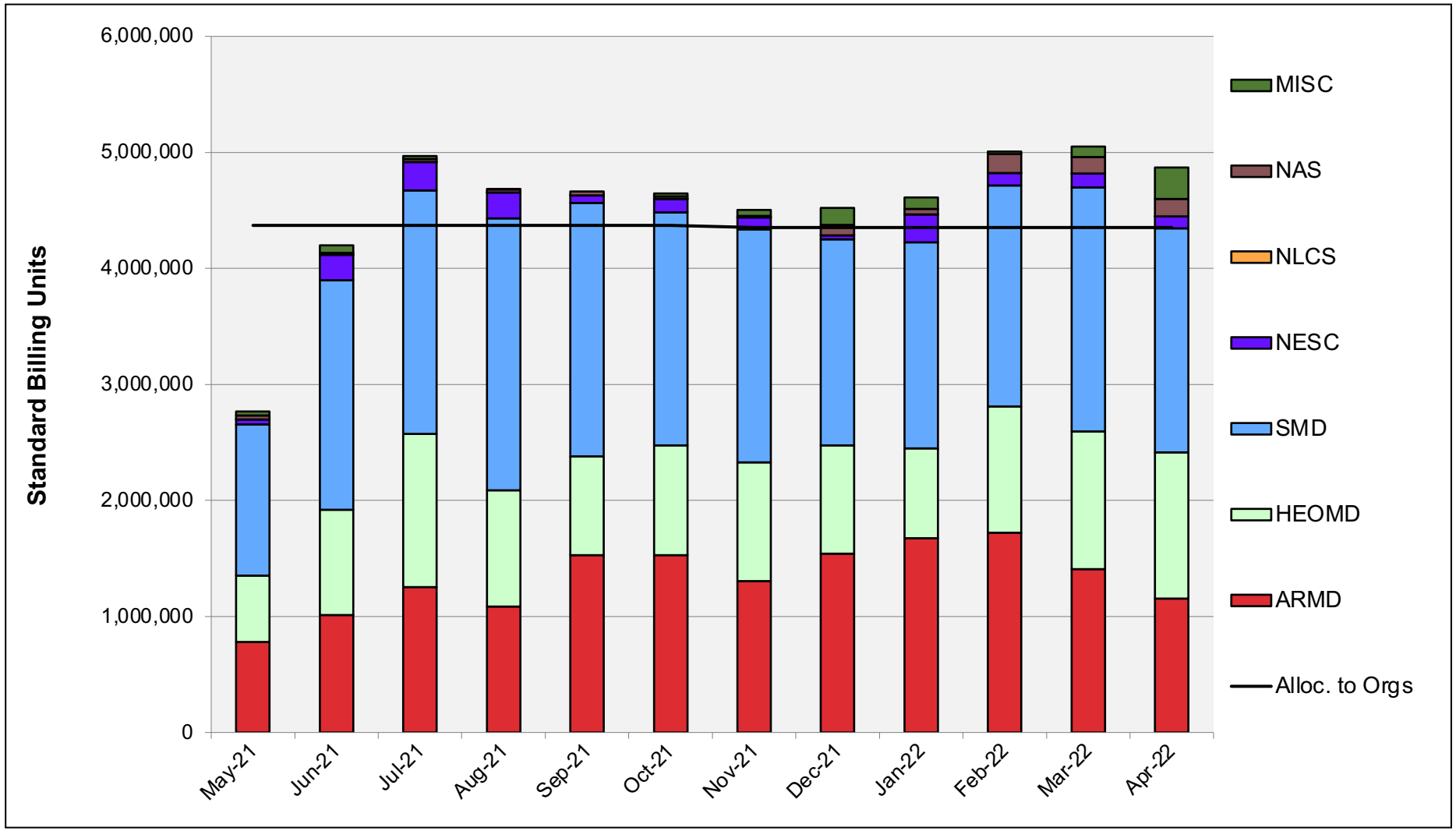
# Aitken: Average Time to Clear All Jobs



# Aitken: Average Expansion Factor



# Pleiades: SBUs Reported, Normalized to 30-Day Month



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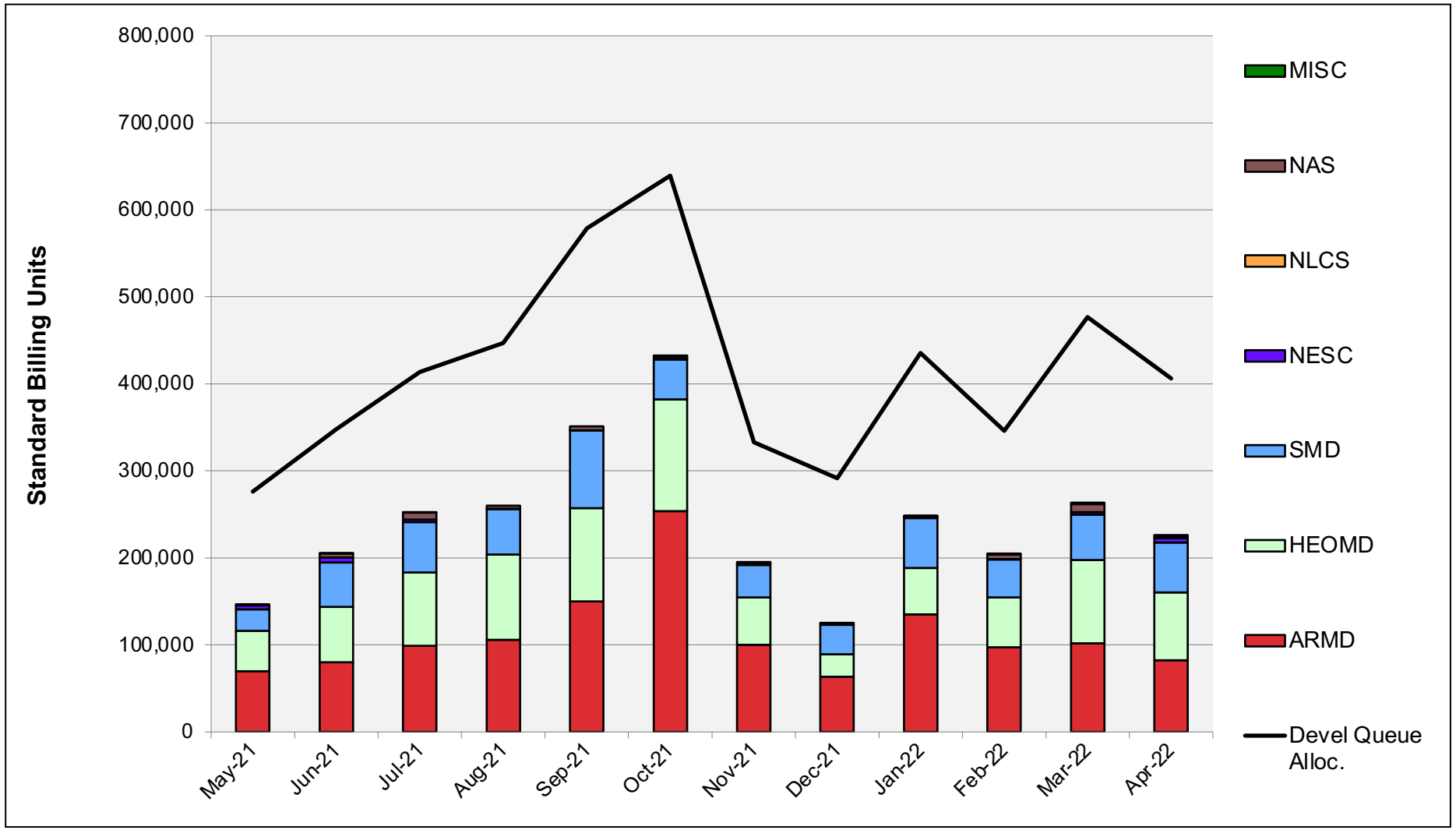

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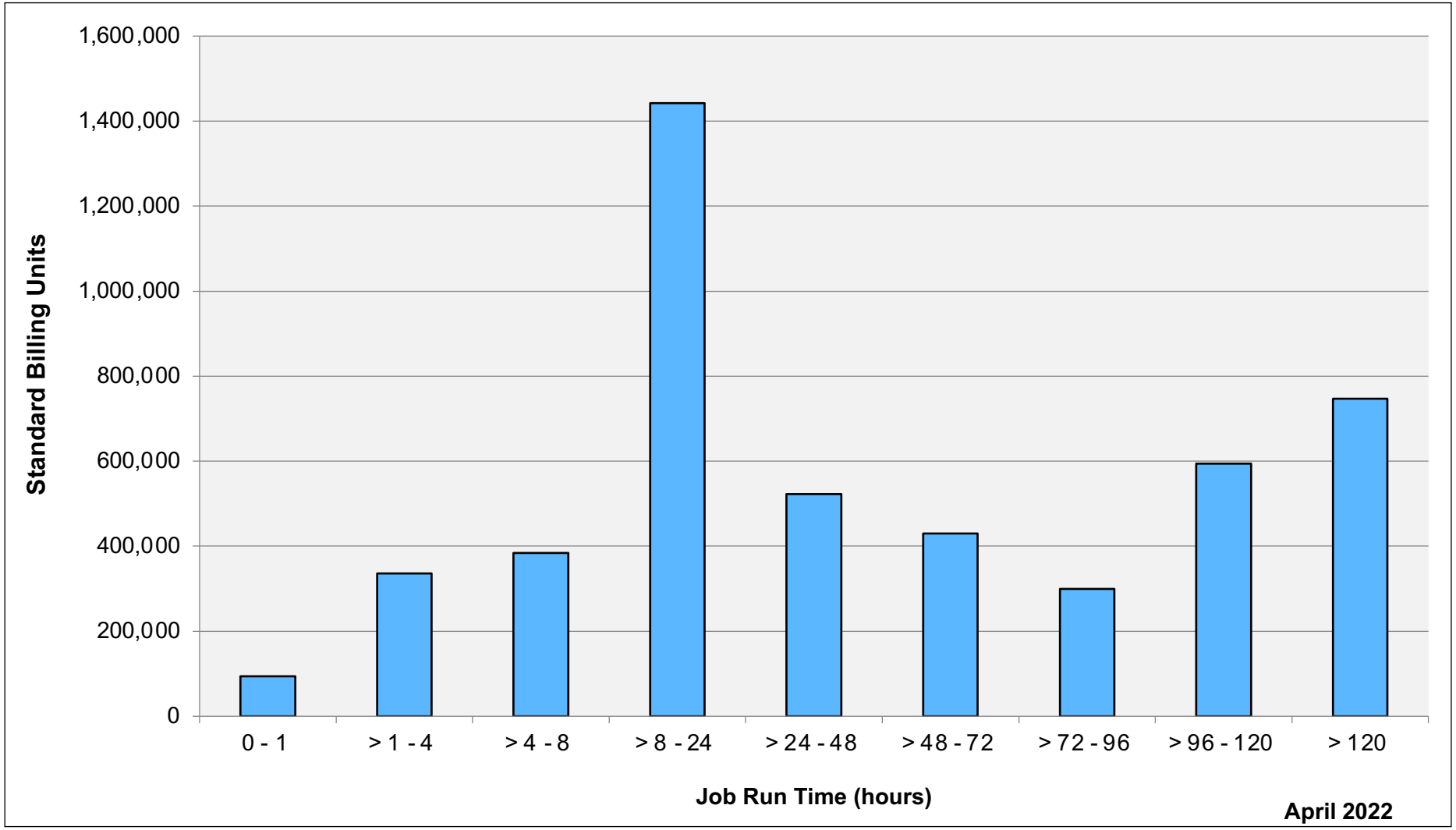

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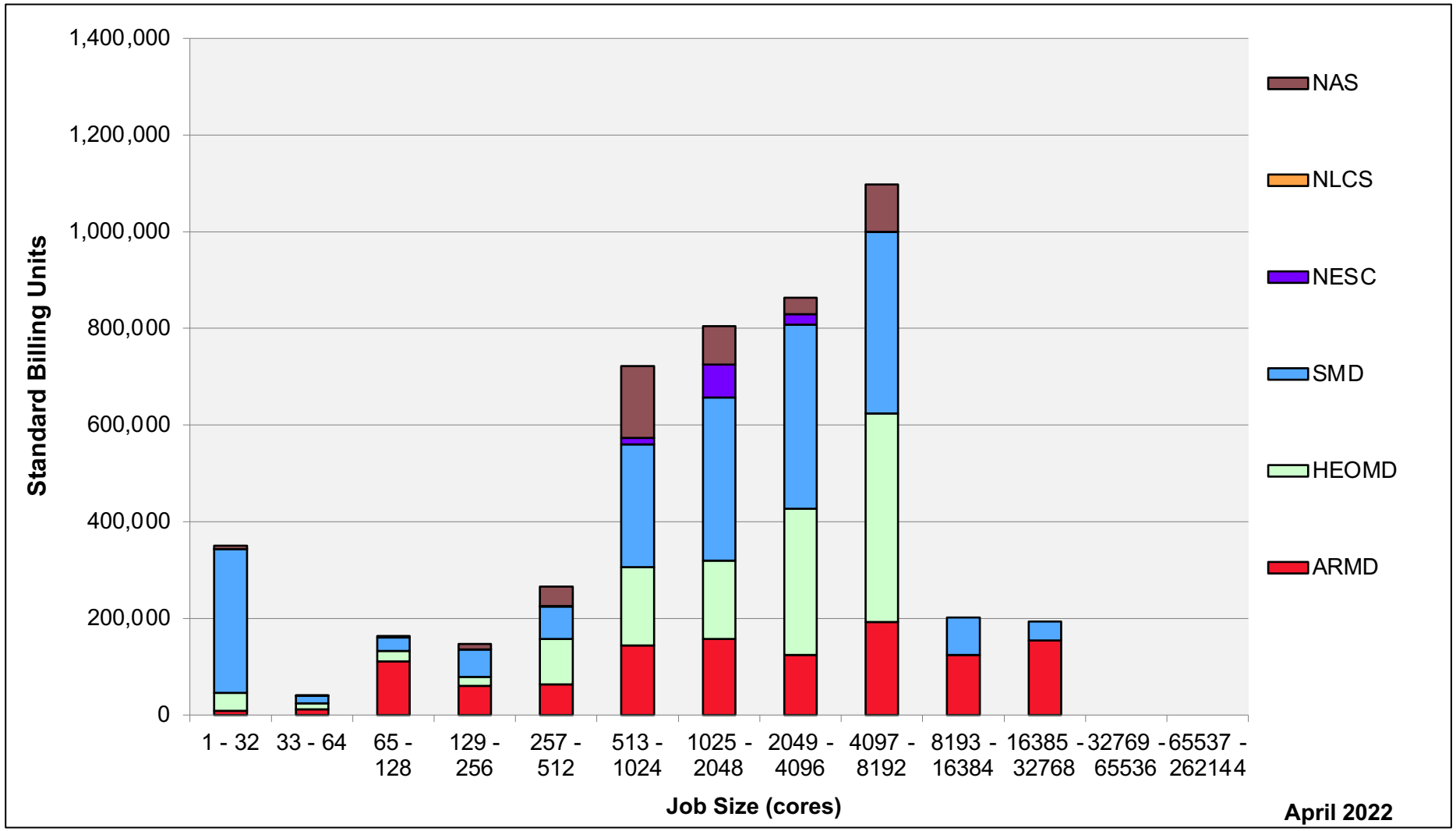

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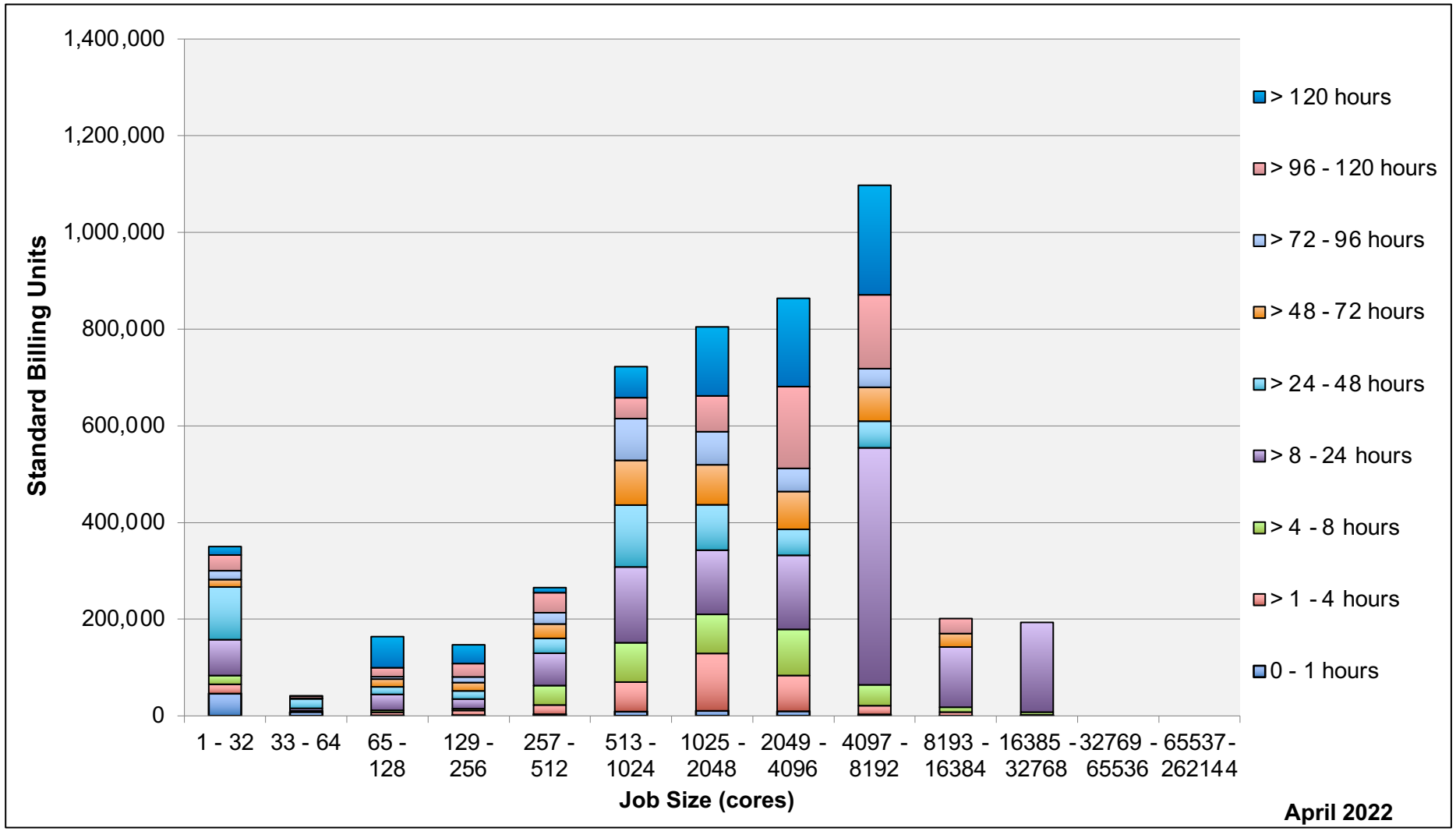

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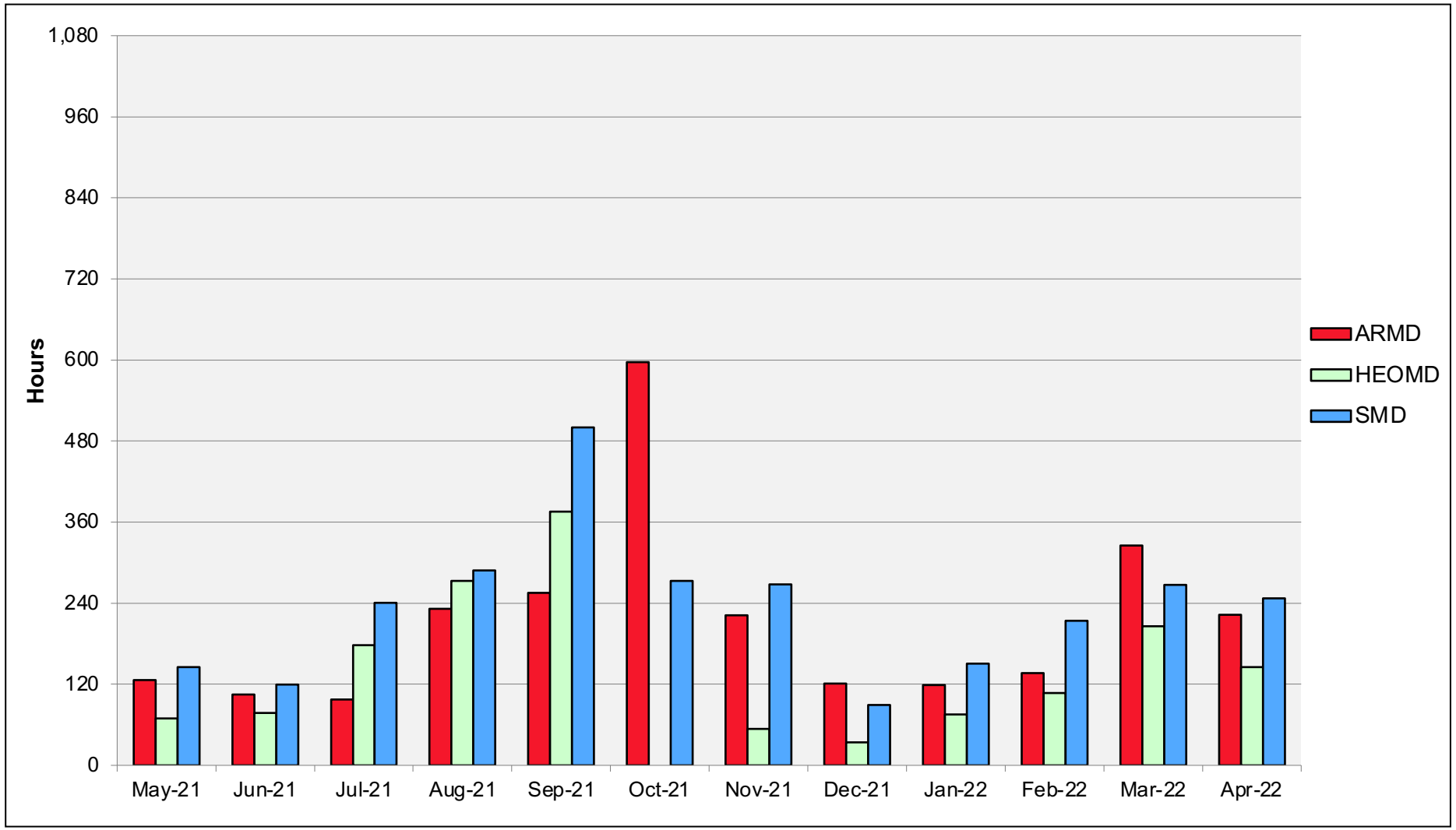
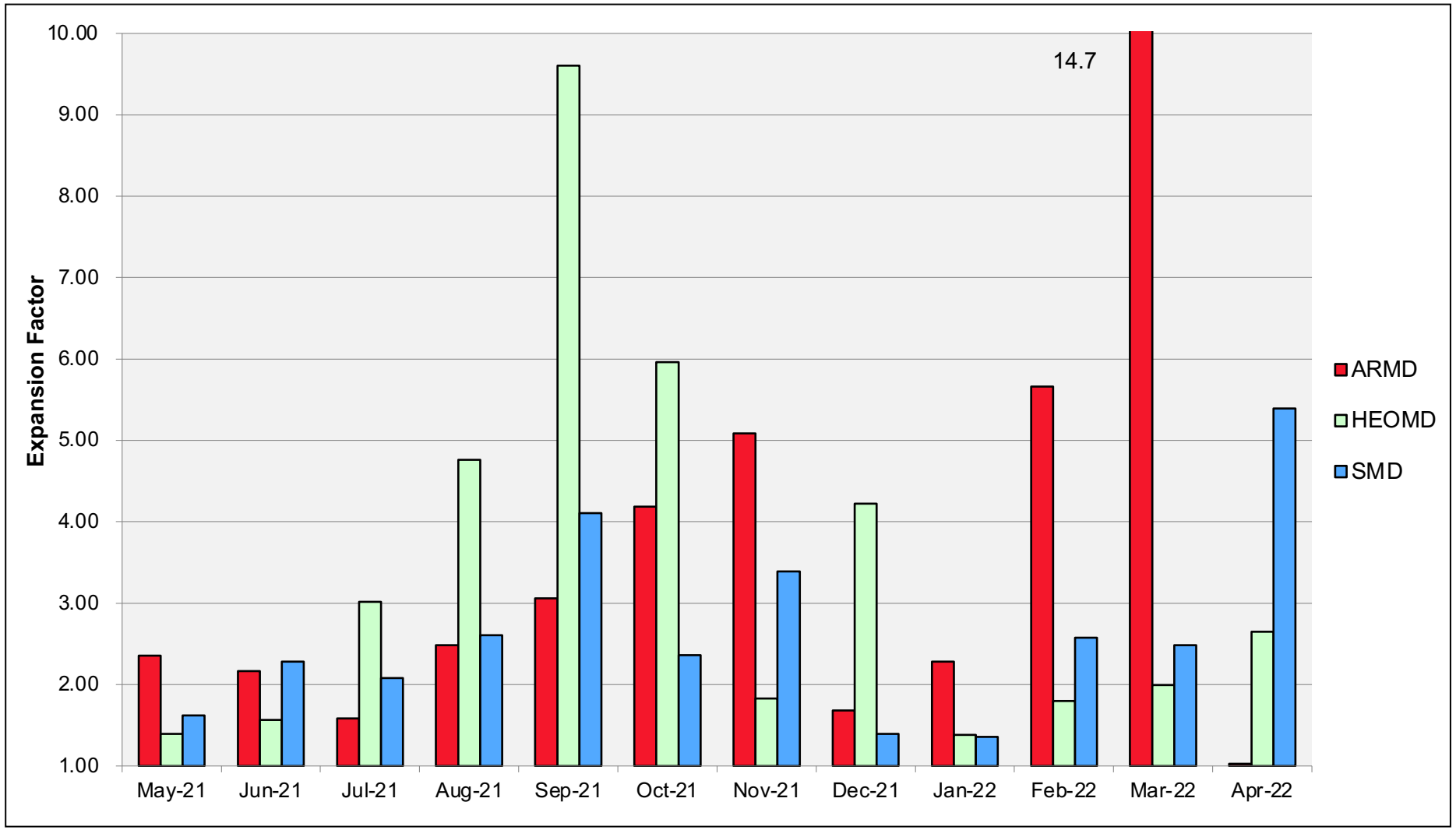
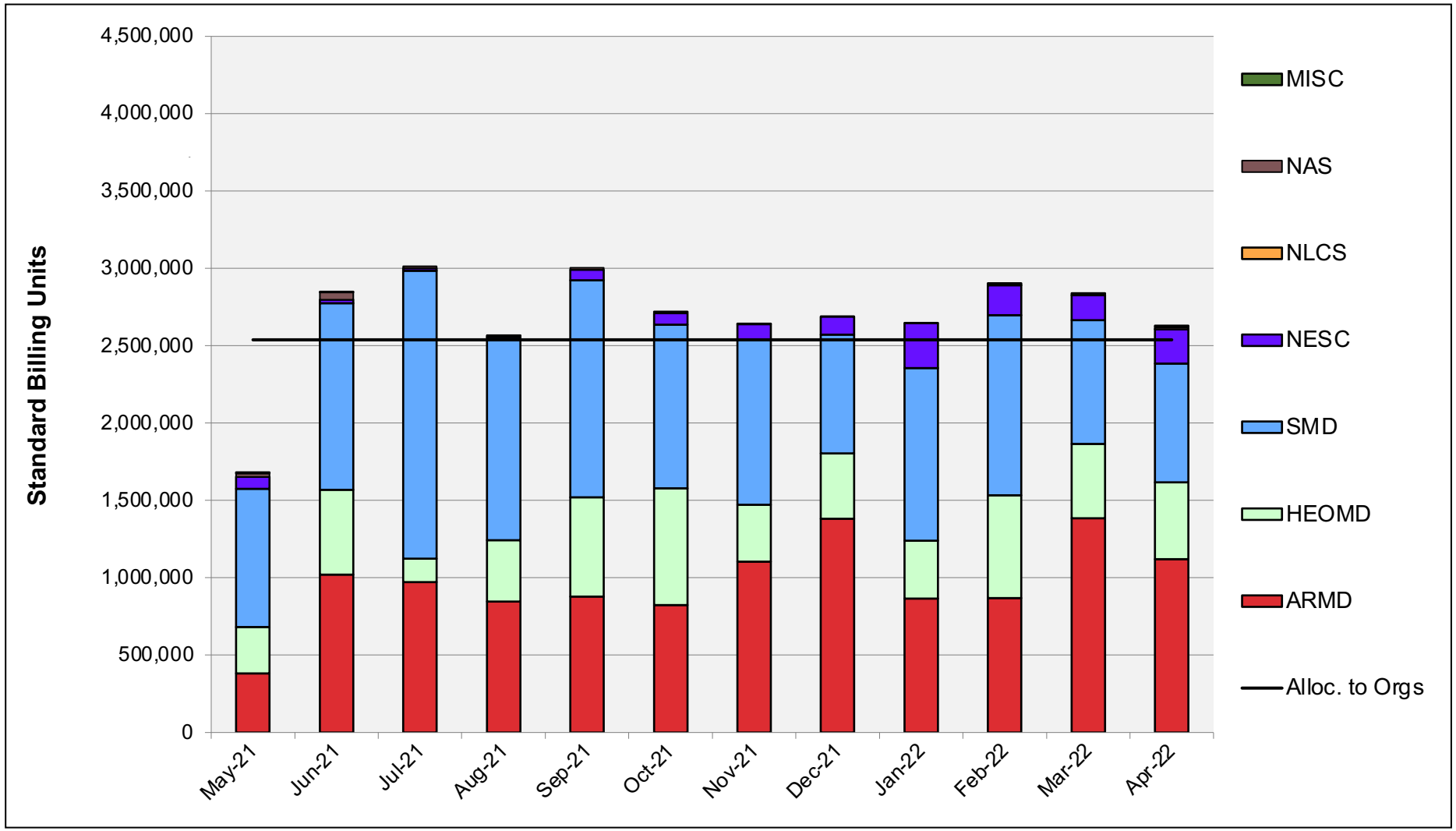


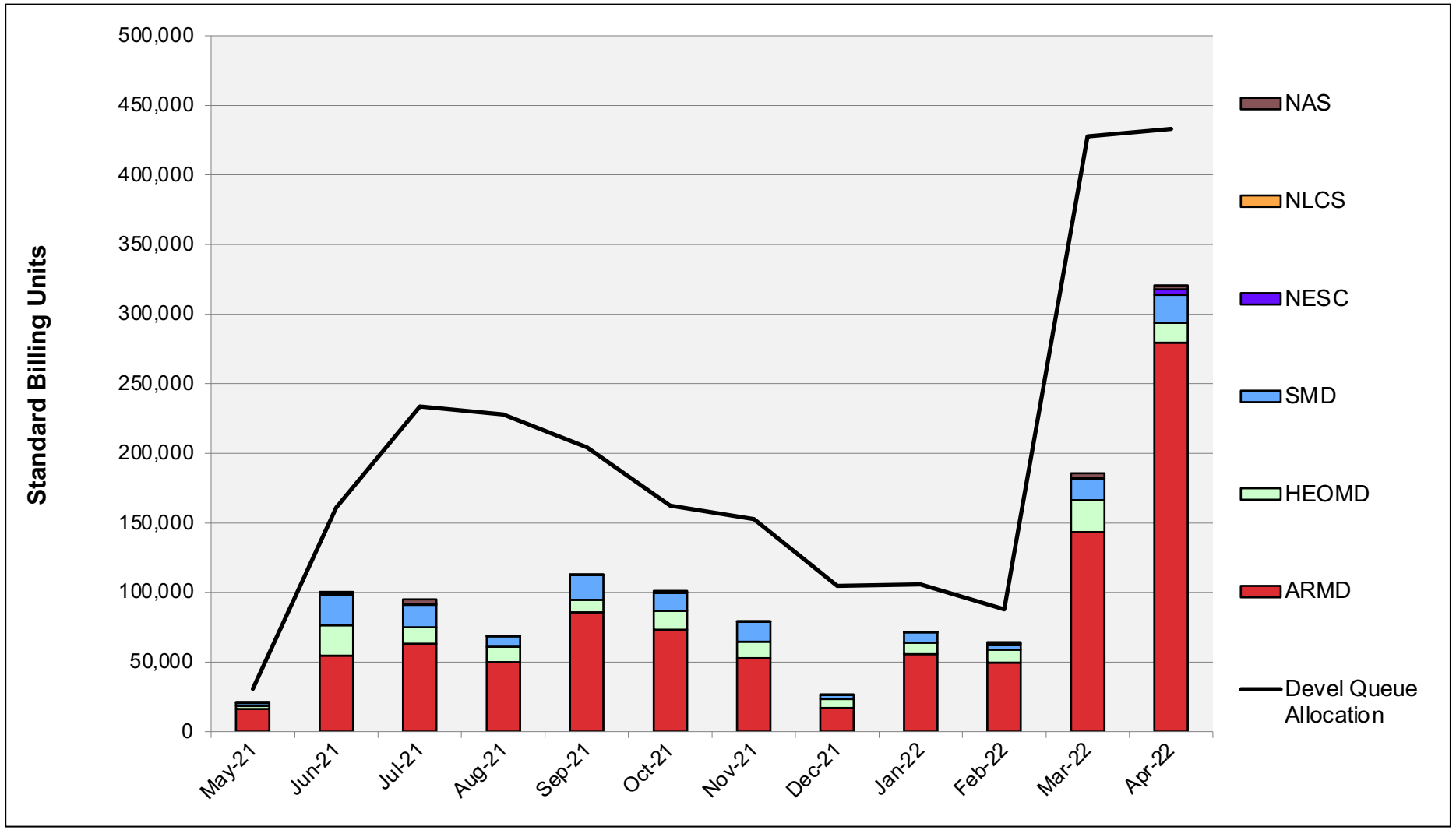
# Pleiades: Average Expansion Factor



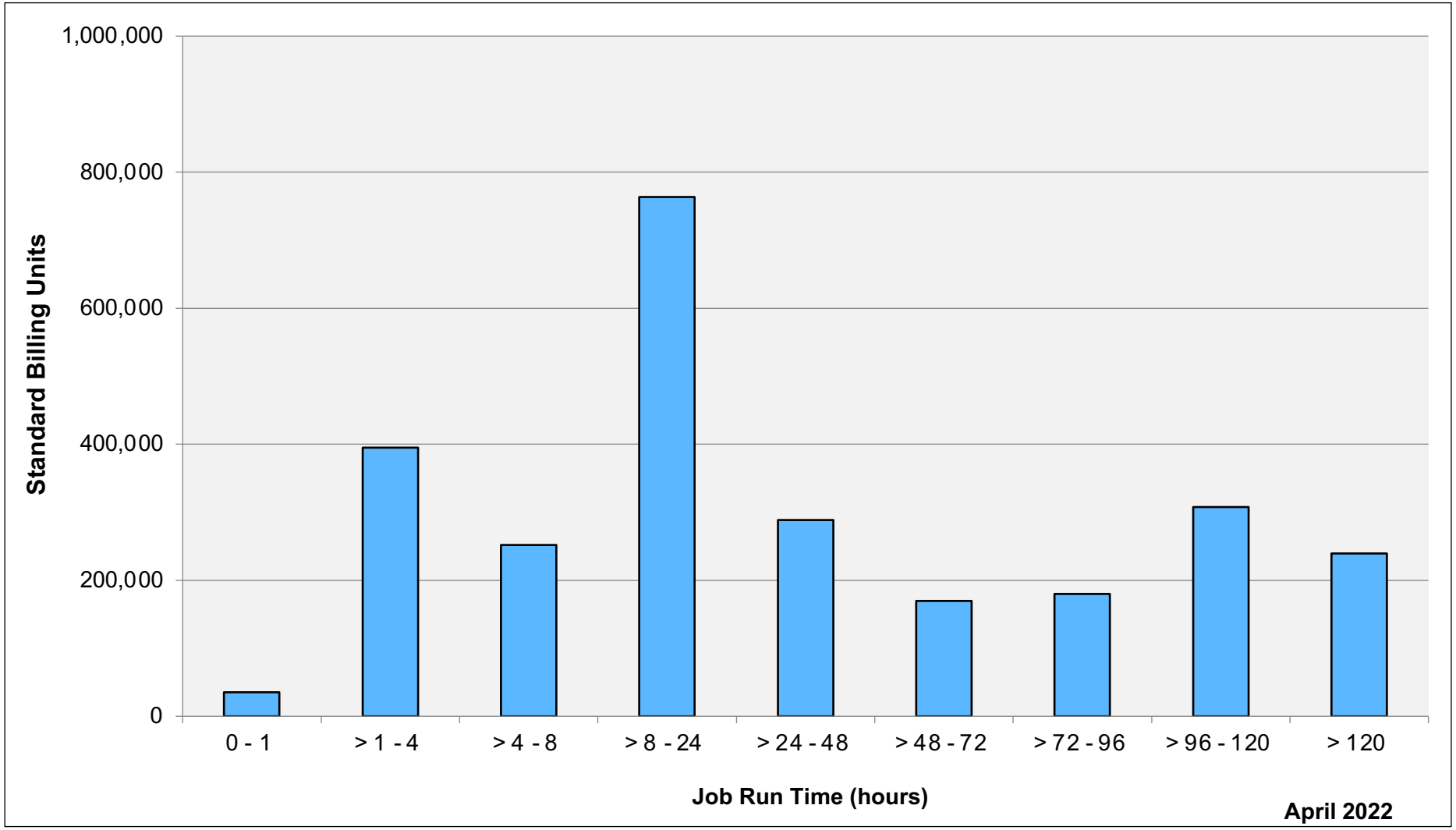
# Electra: SBUs Reported, Normalized to 30-Day Month



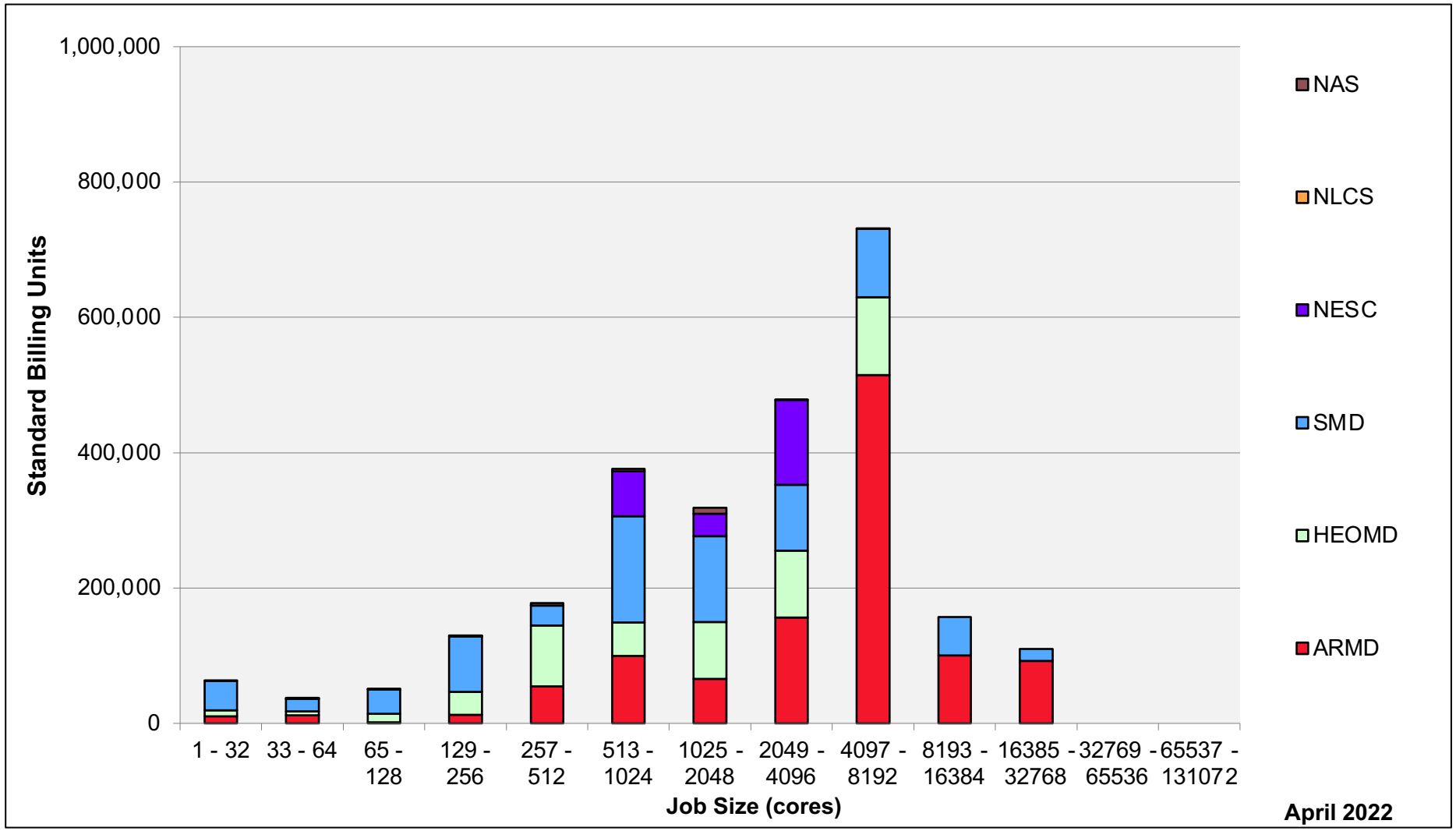
# Electra: Devel Queue Utilization



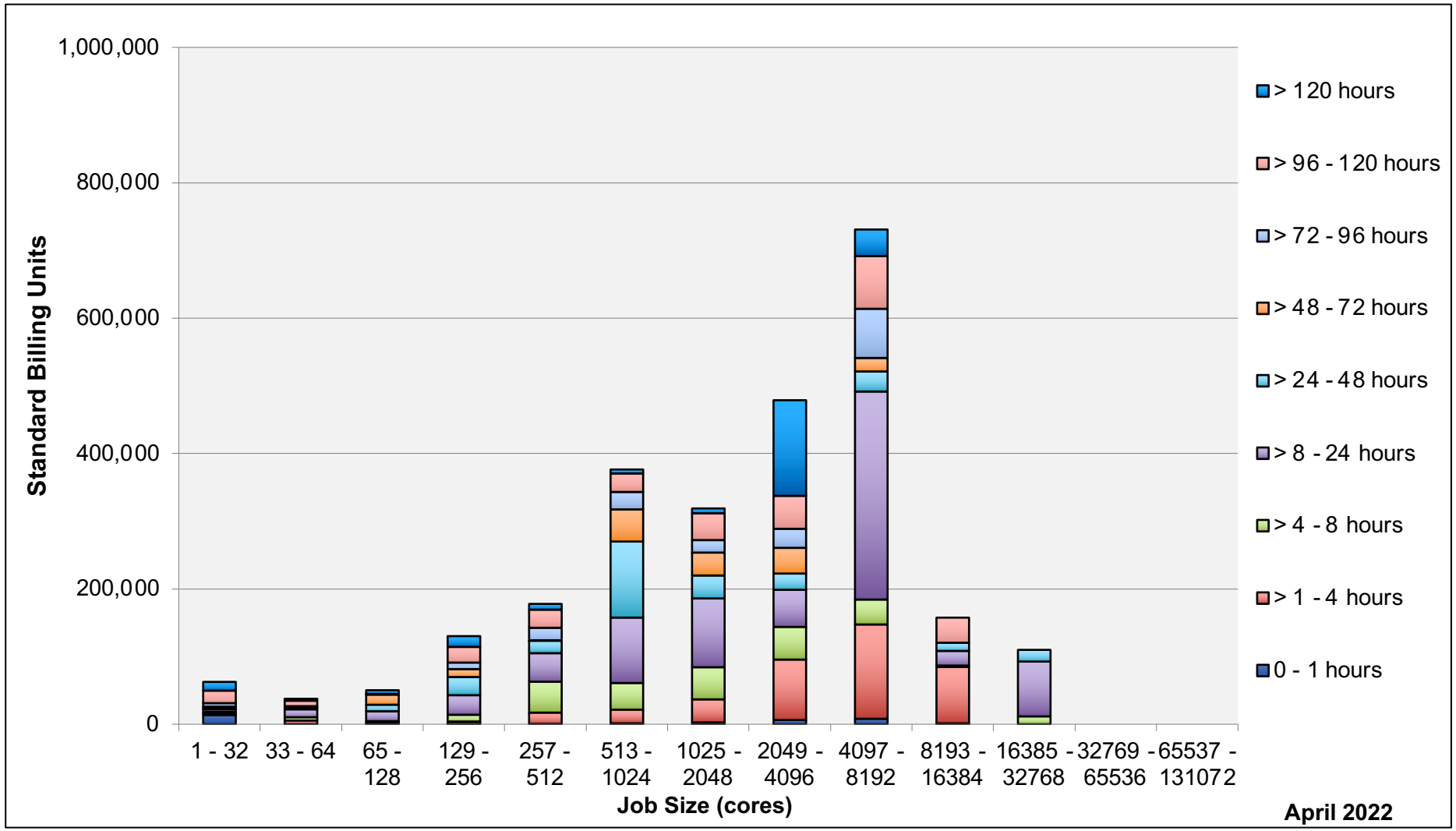
# Electra: Monthly Utilization by Job Length



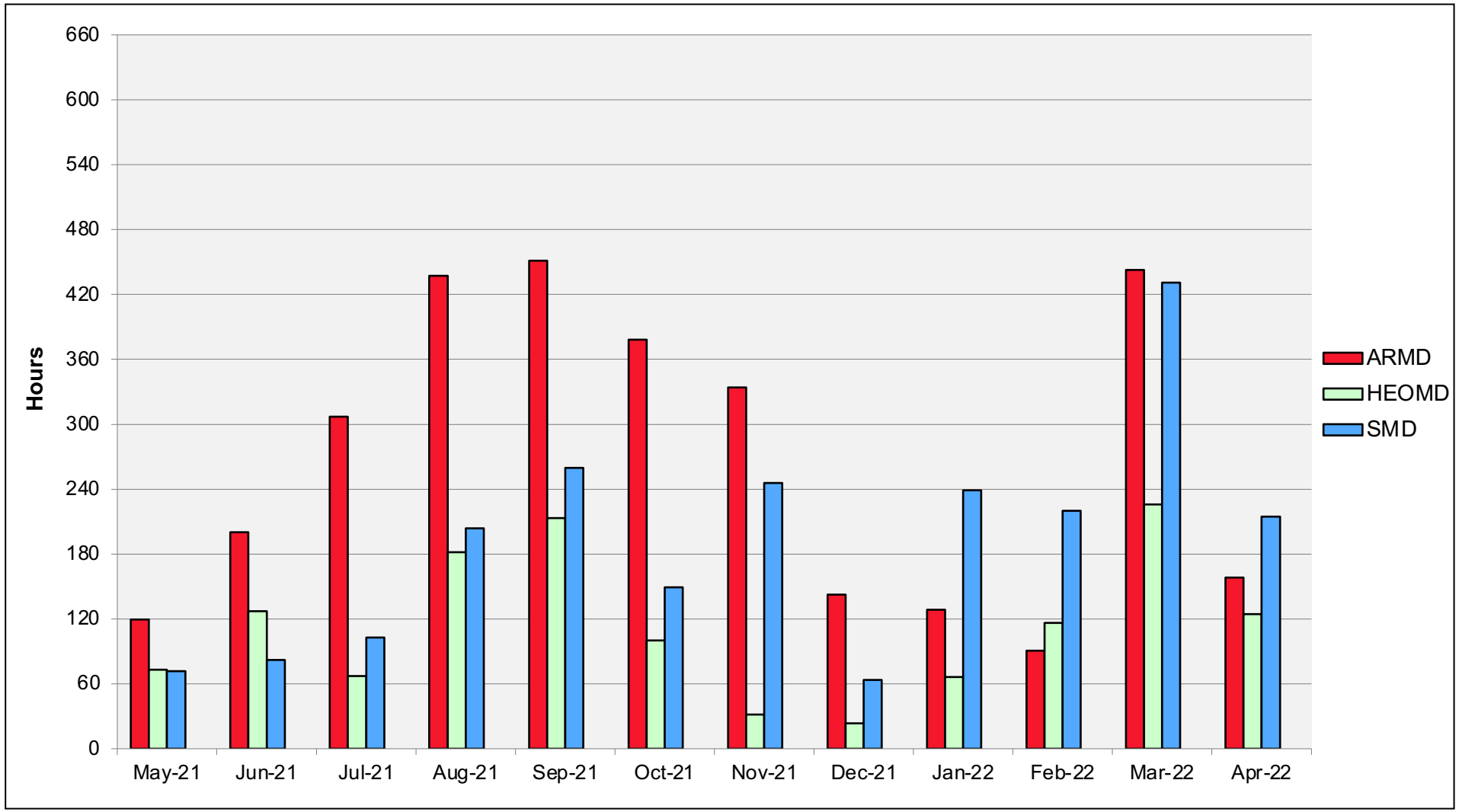
# Electra: Monthly Utilization by Job Size



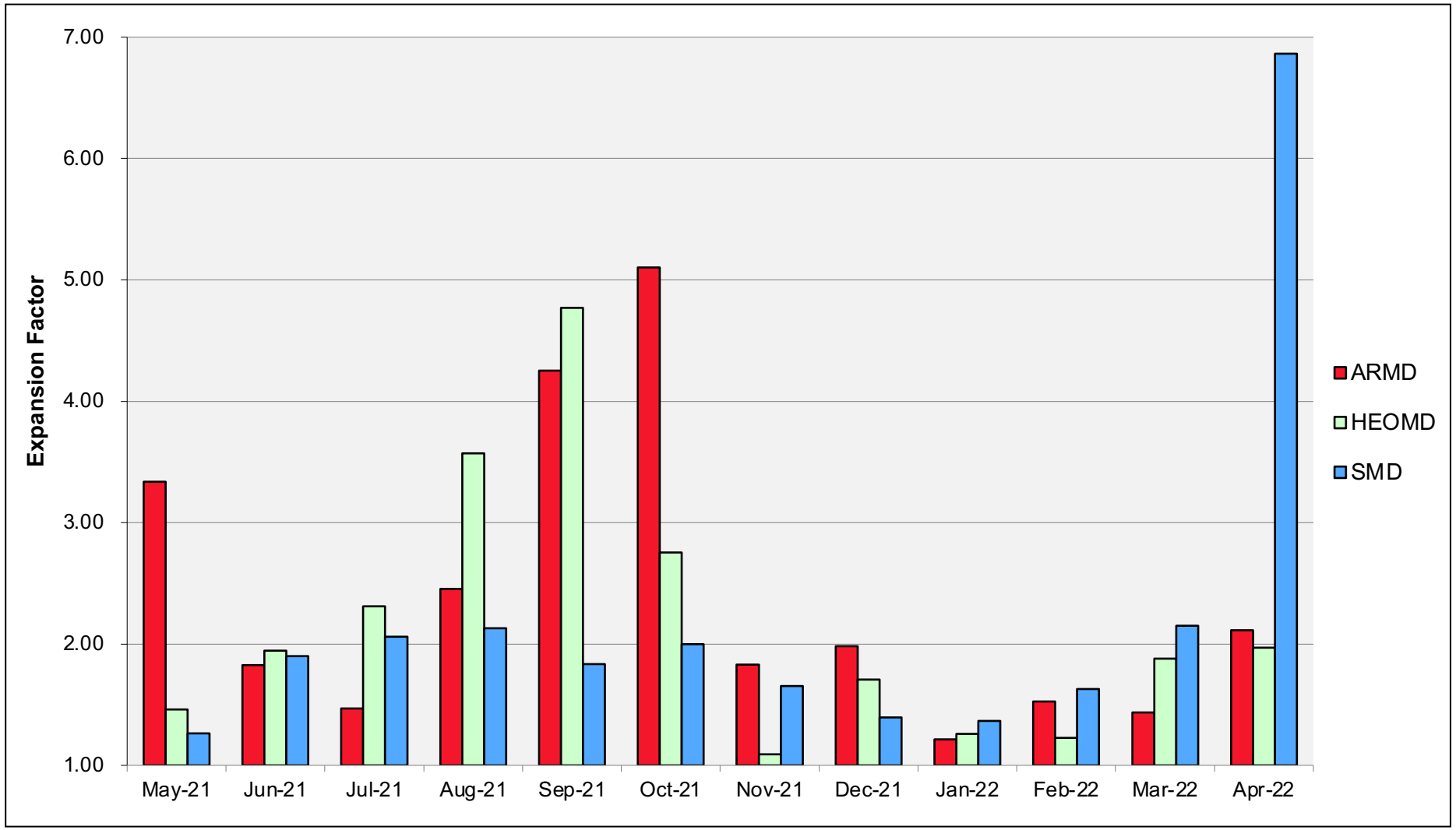
# Electra: Monthly Utilization by Size and Length



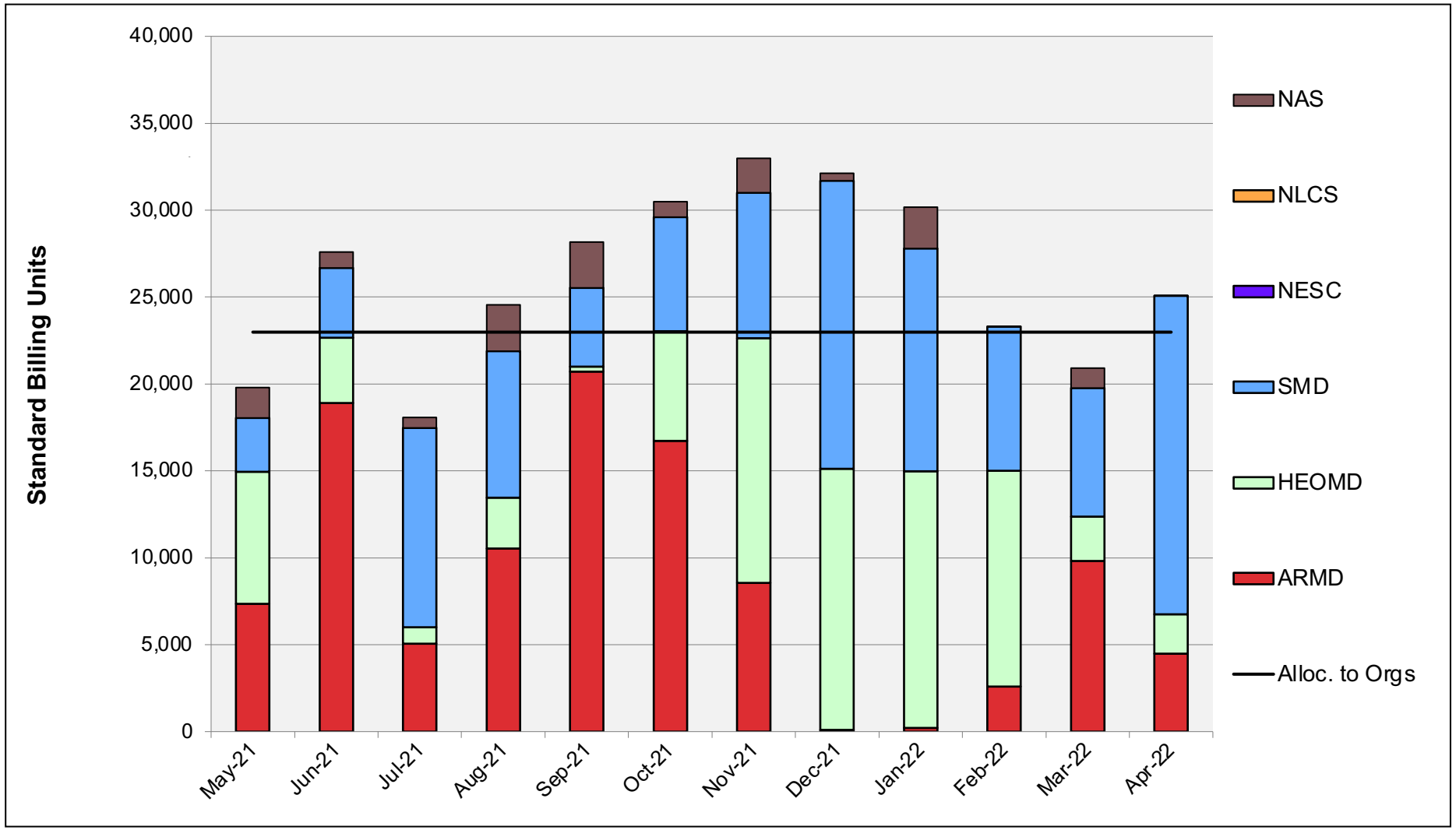
# Electra: Average Time to Clear All Jobs



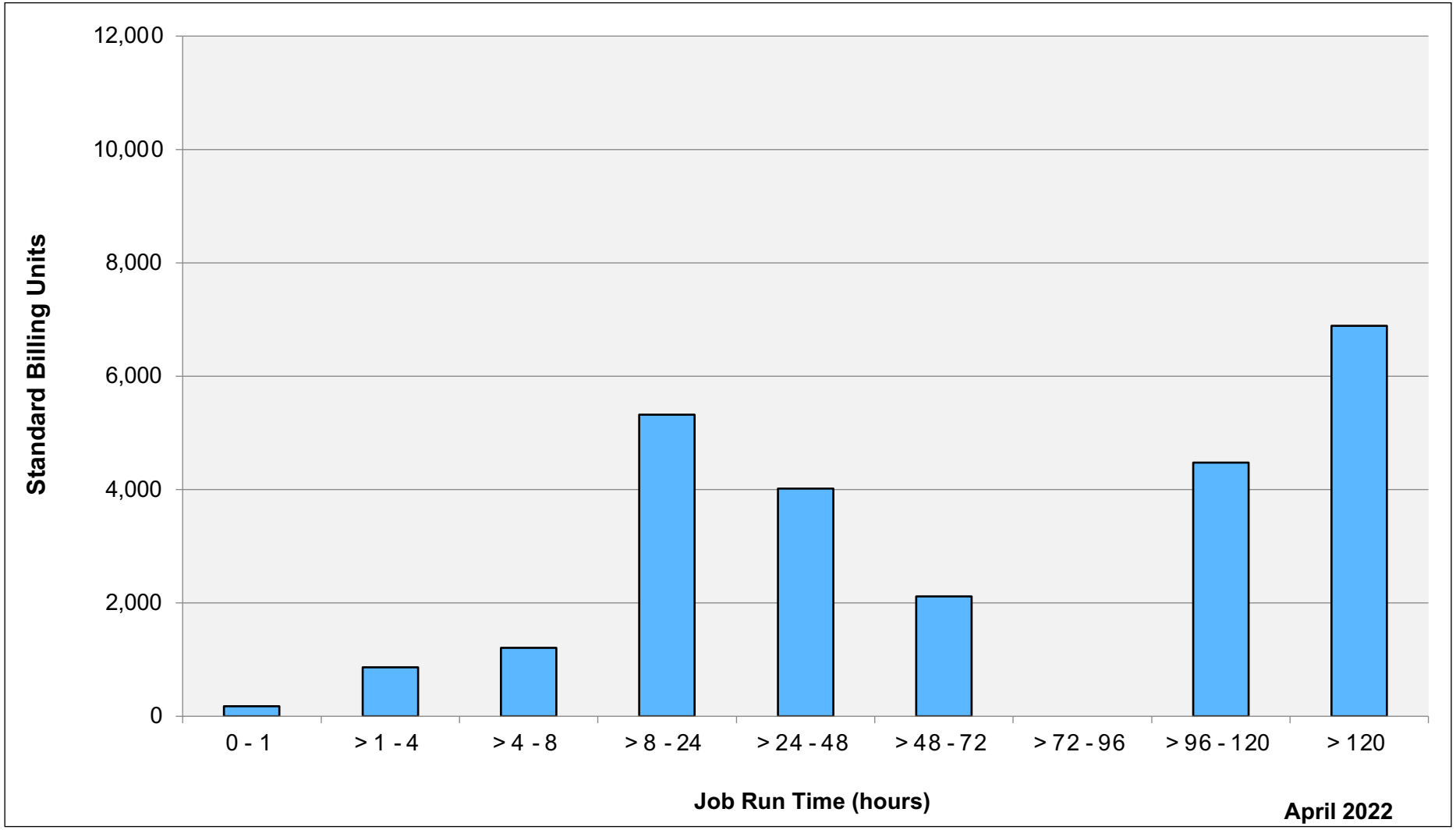
# Electra: Average Expansion Factor



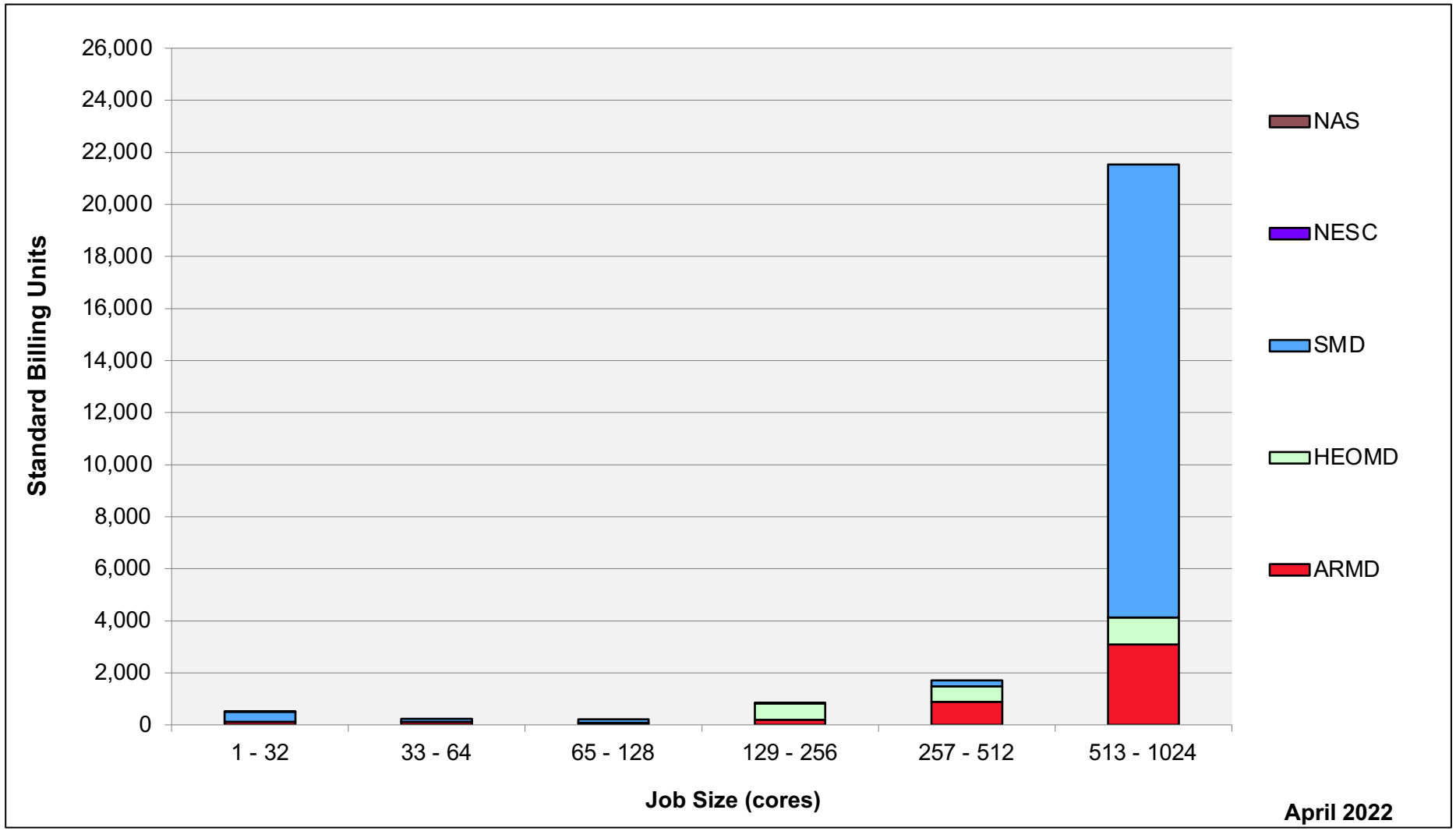
# Endeavour: SBUs Reported, Normalized to 30-Day Month



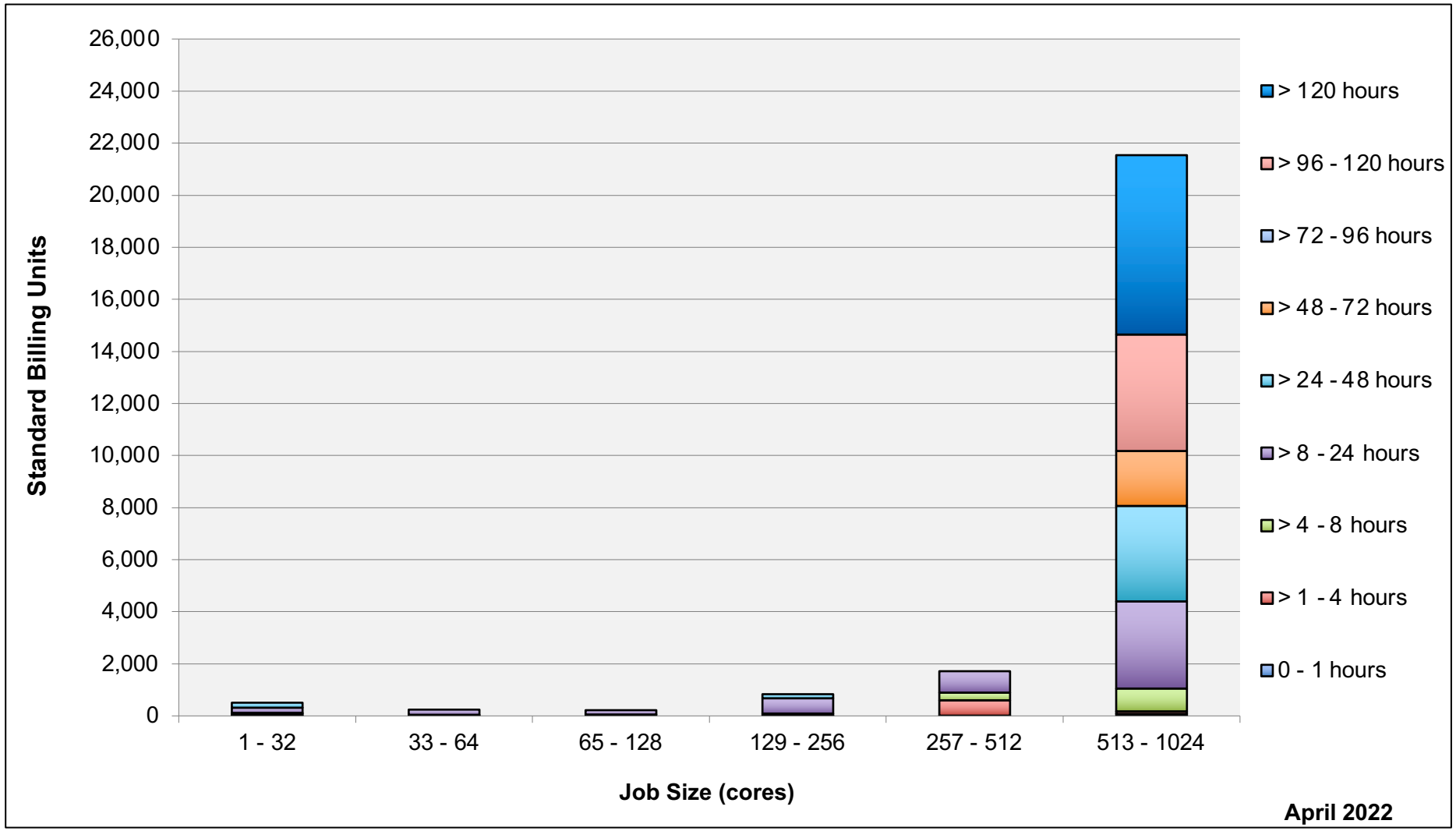
# Endeavour: Monthly Utilization by Job Length



# Endeavour: Monthly Utilization by Job Size



# Endeavour: Monthly Utilization by Size and Length



# Endeavour: Average Expansion Factor